Supporting Information

Simple and efficient copper-catalyzed cascade synthesis of naphthols containing multifunctional groups under mild conditions

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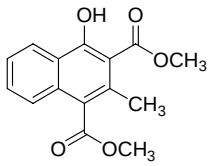
General experimental procedures

All reactions were carried out under nitrogen atmosphere. Proton magnetic resonance spectra (^{1}H NMR) were recorded using tetramethylsilane (TMS) (at 0.00 ppm) in the solvent, remaining $CHCl_3$ in $CDCl_3$ (at 7.26 ppm) or remaining DMSO in DMSO-d_6 (at 2.50 ppm) as the internal standard. Carbon magnetic resonance spectra (^{13}C NMR) were recorded using $CDCl_3$ (at 77.2 ppm) or DMSO-d_6 (at 39.5 ppm) as the internal standard.

Synthesis of compounds 1a-d: Compounds **1a-d** was synthesized according to the known methods.[1,2]

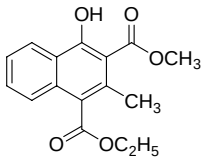
General procedure for synthesis of compounds 3a-t. A 10 mL round bottom flask was charged with a magnetic stirrer and dry DMF (2 mL), substituted methyl 3-(2-halophenyl)-3-oxopropanoate or 3-(2-bromo-5-chlorophenyl)-3-oxopropanenitrile (**1**) (0.5 mmol), *β*-keto ester, acetylacetone, alkyl 2-cyanoacetate, 3-oxo-3-phenylpropanenitrile or malononitrile (**2**) (0.6 mmol), Cs_2CO_3 (1 mmol, 326 mg), after stirring of the mixture for 10 min under nitrogen atmosphere, and CuCl (0.05 mmol, 5 mg) was added to the flask. The mixture was stirred at the shown temperature in Table 2 in text for a time under nitrogen atmosphere. The resulting mixture was filtered, the solid was washed with ethyl acetate two times (2 × 3 mL), and the combined filtrate was concentrated by the rotary evaporator, and the residue was purified by column chromatography on silica gel using petroleum ether/ethyl acetate as eluent to give the desired product.



3a

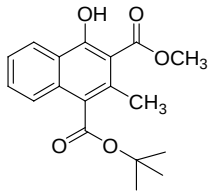
Dimethyl 4-hydroxy-2-methylnaphthalene-1,3-dicarboxylate (3a). Eluent: petroleum ether/ethyl acetate (15:1). Yield 123 mg (90%) using methyl 3-(2-bromophenyl)-3-oxopropanoate as the substrate; 71 mg (52%) using methyl

3-(2-chlorophenyl)-3-oxopropanoate as the substrate. White solid, mp 95-97 °C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 12.79 (s, 1H), 8.41 (d, 1H, *J* = 8.3 Hz), 7.65-7.53 (m, 2H), 7.52-7.45 (m, 1H), 4.01 (s, 3H), 4.00 (s, 3H) , 2.57 (s, 3H). ^{13}C NMR ($CDCl_3$, 75MHz) δ 172.9, 170.6, 163.0, 132.7, 132.6, 130.7, 125.8, 124.4, 124.1, 123.5, 106.1, 52.6, 52.5, 21.2. HR-MS $[M-H]^-$ m/z Calcd for $C_{15}H_{13}O_5$: 273.0763. Found: 273.0755.



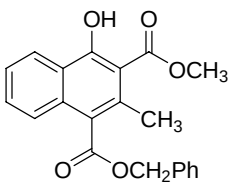
3b

1-Ethyl 3-methyl 4-hydroxy-2-methylnaphthalene-1,3-dicarboxylate (3b). Eluent: petroleum ether/ethyl acetate (15:1). Yield 95 mg (66%). White solid, mp 86-88 °C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 12.77 (s, 1H), 8.40 (d, 1H, *J* = 8.3 Hz), 7.64-7.59 (m, 2H), 7.52-7.44 (m, 1H), 4.50 (q, 2H, *J* = 7.2 Hz), 4.00 (s, 3H), 2.58 (s, 3H), 1.44 (t, 3H, *J* = 7.2 Hz). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 172.9, 170.1, 162.9, 132.6, 132.5, 130.7, 125.7, 124.8, 124.4, 124.1, 123.5, 106.1, 61.5, 52.6, 21.0, 14.4. HR-MS $[M-H]^-$ m/z Calcd for $C_{16}H_{15}O_5$: 287.0919. Found: 287.0913.



3c

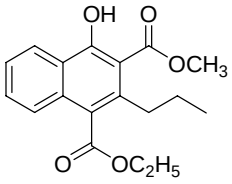
1-*tert*-Butyl 3-methyl 4-hydroxy-2-methylnaphthalene-1,3-dicarboxylate (3c). Eluent: petroleum ether/ethyl acetate (15:1). Yield 119 mg (75%). White solid, mp 161-163 °C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 12.71 (s, 1H), 8.40 (d, 1H, *J* = 8.3 Hz), 7.71-7.58 (m, 2H), 7.52-7.44 (m, 1H), 4.00 (s, 3H), 2.61 (s, 3H), 1.67 (s, 9H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 173.0, 169.4, 162.6, 132.6, 131.6, 130.6, 126.1, 125.6, 124.4, 124.0, 123.5, 106.1, 82.4, 52.5, 28.4, 20.7. HR-MS $[M-H]^-$ m/z Calcd for $C_{18}H_{19}O_5$: 315.1232. Found: 315.1228.



3d

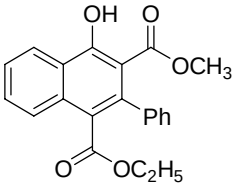
1-Benzyl 3-methyl 4-hydroxy-2-methylnaphthalene-1,3-dicarboxylate (3d). Eluent:

petroleum ether/ethyl acetate (10:1). Yield 166 mg (95%). White solid, mp 96-97 °C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 12.78 (s, 1H), 8.39 (d, 1H, *J* = 8.4 Hz), 7.57-7.34 (m, 8H), 5.47 (s, 2H), 3.98 (s, 3H), 2.53 (s, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 172.9, 169.9, 163.1, 135.6, 132.7, 132.6, 130.7, 128.8, 128.7, 128.6, 125.7, 124.4, 124.3, 124.1, 123.5, 106.1, 67.4, 52.6, 21.1. HR-MS $[M-H]^-$ m/z Calcd for $C_{21}H_{17}O_5$: 349.1076. Found: 349.1076.



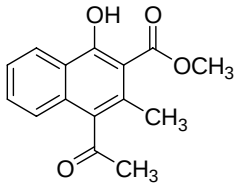
3e

1-Ethyl 3-methyl 4-hydroxy-2-propylnaphthalene-1,3-dicarboxylate (3e). Eluent: petroleum ether/ethyl acetate (15:1). Yield 107 mg (68%). White solid, mp 57-59 °C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 12.76 (s, 1H), 8.41 (d, 1H, *J* = 8.6 Hz), 7.65-7.55 (m, 2H), 7.52-7.44 (m, 1H), 4.51 (q, 2H, *J* = 7.2 Hz), 4.02 (s, 3H), 2.96 (t, 2H, *J* = 7.9 Hz), 1.69-1.54 (m, 2H), 1.44 (t, 2H, *J* = 6.9 Hz), 0.98 (t, 3H, *J* = 7.2 Hz). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 172.8, 170.1, 163.2, 136.9, 132.6, 130.6, 125.8, 124.7, 124.5, 124.2, 123.7, 105.3, 61.5, 52.7, 36.0, 25.4, 14.8, 14.5. HR-MS $[M-H]^-$ m/z Calcd for $C_{18}H_{19}O_5$: 315.1232. Found: 315.1230.



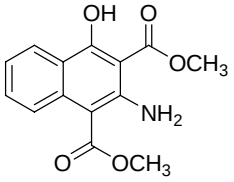
3f

1-Ethyl 3-methyl 4-hydroxy-2-phenylnaphthalene-1,3-dicarboxylate (3f). Eluent: petroleum ether/ethyl acetate (15:1). Yield 158 mg (90%). White solid, mp 123-125 °C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 12.46 (s, 1H), 8.49 (d, 1H, *J* = 8.3 Hz), 7.80 (d, 1H, *J* = 8.3 Hz), 7.72-7.63 (m, 1H), 7.62-7.54 (m, 1H), 7.37-7.22 (m, 5H), 3.99 (q, 2H, *J* = 7.2 Hz), 3.45 (s, 3H), 0.90 (t, 3H, *J* = 7.2 Hz). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 172.1, 168.9, 162.1, 140.7, 137.2, 132.3, 130.9, 128.9, 127.4, 127.1, 126.5, 125.1, 124.8, 124.4, 124.1, 105.7, 61.3, 52.1, 13.8. HR-MS $[M-H]^-$ m/z Calcd for $C_{21}H_{17}O_5$: 349.1076. Found: 349.1075.



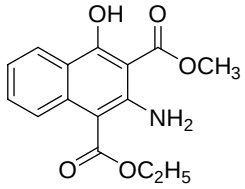
3g

Methyl 4-acetyl-1-hydroxy-3-methyl-2-naphthoate (3g). Eluent: petroleum ether/ethyl acetate (10:1). Yield 123 mg (95%). White solid, mp 124-126 °C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 12.74 (s, 1H), 8.43 (d, 1H, *J* = 8.3 Hz), 7.65-7.57 (m, 1H), 7.54-7.44 (m, 2H), 4.02 (s, 3H), 2.59 (s, 3H), 2.53 (s, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 208.4, 173.0, 162.6, 132.3, 131.7, 130.7, 129.5, 125.7, 124.7, 123.7, 123.6, 106.1, 52.6, 33.7, 20.6. HR-MS $[M-H]^-$ m/z Calcd for $C_{15}H_{13}O_4$: 257.0814. Found: 257.0808.



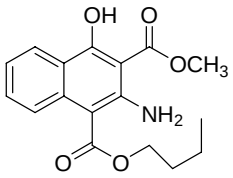
3h

Dimethyl 2-amino-4-hydroxynaphthalene-1,3-dicarboxylate (3h).[3] Eluent: petroleum ether/ethyl acetate (4:1). Yield 84 mg (61%). Yellow solid, mp 129-131 °C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 13.27 (s, 1H), 8.30-8.21 (m, 2H), 7.77 (s, 2H), 7.54-7.47 (m, 1H), 7.23-7.15 (m, 1H), 4.08 (s, 3H) , 3.96 (s, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 171.9, 170.3, 167.5, 151.0, 136.8, 131.6, 124.8, 124.7, 122.0, 119.0, 96.5, 96.3, 53.1, 51.4. HR-MS $[M-H]^-$ m/z Calcd for $C_{14}H_{12}NO_5$: 274.0716. Found: 274.0718.



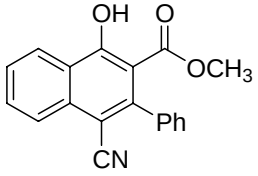
3i

1-Ethyl 3-methyl 2-amino-4-hydroxynaphthalene-1,3-dicarboxylate (3i). Eluent: petroleum ether/ethyl acetate (4:1). Yield 151 mg (66%). Yellow solid, mp 69-70 °C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 13.21 (s, 1H), 8.30-8.20 (m, 2H), 7.67 (s, 2H), 7.52-7.43 (m, 1H), 7.20-7.12 (m, 1H), 4.44 (q, 2H, *J* = 7.2 Hz), 4.00 (s, 3H), 1.44 (t, 3H, *J* = 7.2 Hz). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 171.9, 169.8, 167.3, 150.8, 136.8, 131.5, 124.7, 124.6, 121.9, 118.9, 96.8, 96.3, 60.5, 53.0, 14.6. HR-MS $[M-H]^-$ m/z Calcd for $C_{15}H_{14}NO_5$: 288.0872. Found: 288.0876.



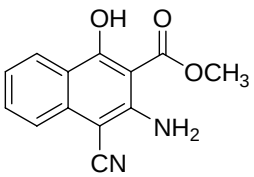
3j

1-Butyl 3-methyl 2-amino-4-hydroxynaphthalene-1,3-dicarboxylate (3j). Eluent: petroleum ether/ethyl acetate (4:1). Yield 102 mg (64%) using methyl 3-(2-bromophenyl)-3-oxopropanoate as the substrate; 92 mg (58%) using methyl 3-(2-chlorophenyl)-3-oxopropanoate as the substrate. Yellow solid, mp 58-61 ^{o}C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 13.25 (s, 1H), 8.31-8.23 (m, 2H), 7.71 (s, 2H), 7.53-7.46 (m, 1H), 7.22-7.15 (m, 1H), 4.39 (t, 2H, J = 6.9 Hz), 4.08 (s, 3H), 1.86-1.74 (m, 2H), 1.58-1.43 (m, 2H), 0.99 (t, 3H, J = 7.2 Hz). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 172.0, 170.0, 168.4, 150.8, 136.9, 131.5, 124.8, 124.7, 122.0, 119.0, 96.9, 96.3, 64.6, 53.1, 31.0, 19.7, 13.9. HR-MS $[M-H]^-$ m/z Calcd for $C_{17}H_{18}NO_5$: 316.1185. Found: 316.1178.



3k

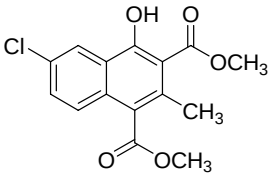
Methyl 4-cyano-1-hydroxy-3-phenyl-2-naphthoate (3k). Eluent: petroleum ether/ethyl acetate (10:1). Yield 96 mg (63%) using methyl 3-(2-bromophenyl)-3-oxopropanoate as the substrate; 62 mg (41%) using methyl 3-(2-chlorophenyl)-3-oxopropanoate as the substrate. White solid, mp 153-154 ^{o}C. ^{1}H NMR ($CDCl_3$, 600 MHz) δ 8.51 (d, 1H, J = 6.9 Hz), 8.20 (d, 1H, J = 6.9 Hz), 7.83 (s, 1H), 7.67 (s, 1H), 7.52-7.39 (m, 3H), 7.36-7.28 (m, 2H), 3.49 (s, 3H). ^{13}C NMR ($CDCl_3$, 150 MHz) δ 171.4, 164.6, 147.4, 139.7, 134.5, 132.3, 128.4, 128.3, 128.0, 127.4, 125.4, 124.7, 124.0, 117.0, 106.4, 103.4, 52.5. HR-MS $[M-H]^-$ m/z Calcd for $C_{19}H_{12}NO_3$: 302.0817. Found: 302.0809.



3l

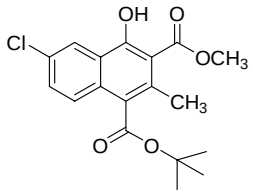
Methyl 3-amino-4-cyano-1-hydroxy-2-naphthoate (3l). Eluent: petroleum

ether/ethyl acetate (4:1). Yield 101 mg (83%). Light yellow solid, mp 198-200 °C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 13.20 (s, 1H), 8.21 (d, 1H, *J* = 8.3 Hz), 7.74 (d, 1H, *J* = 8.3 Hz), 7.65-7.56 (m, 1H), 7.32-7.21 (m, 1H), 6.12 (s, 2H), 4.09 (s, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 171.2, 167.7, 150.9, 136.4, 132.8, 125.1, 123.3, 122.8, 118.7, 117.9, 96.0, 80.6, 53.4. HR-MS $[M-H]^-$ m/z Calcd for $C_{13}H_9N_2O_3$: 241.0613. Found: 241.0610.



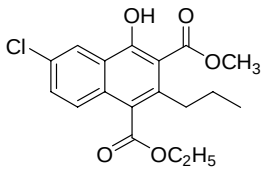
3m

Dimethyl 6-chloro-4-hydroxy-2-methylnaphthalene-1,3-dicarboxylate (3m). Eluent: petroleum ether/ethyl acetate (10:1). Yield 130 mg (84%). White solid, mp 117-119 °C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 12.72 (s, 1H), 8.36 (s, 1H), 7.56-7.50 (m, 2H), 4.01 (s, 3H), 4.00 (s, 3H), 2.55 (s, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 172.6, 170.1, 161.9, 133.3, 131.9, 131.3, 130.8, 125.9, 124.3, 123.6, 107.1, 52.8, 52.6, 21.2. HR-MS $[M-H]^-$ m/z Calcd for $C_{15}H_{12}ClO_5$: 307.0373. Found: 307.0373.



3n

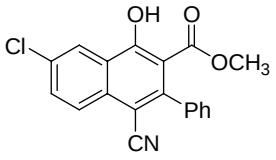
1-*tert*-butyl 3-methyl 6-chloro-4-hydroxy-2-methylnaphthalene-1,3-dicarboxylate (3n). Eluent: petroleum ether/ethyl acetate (10:1). Yield 119 mg (68%). White solid, mp 126-128 °C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 12.65 (s, 1H), 8.36 (s, 1H), 7.65-7.50 (m, 2H), 4.01 (s, 3H), 2.60 (s, 3H), 1.67 (s, 9H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 172.7, 168.9, 161.5, 132.1, 131.7, 130.8, 125.9, 125.8, 124.3, 123.5, 107.0, 82.7, 52.7, 28.4, 20.7. HR-MS $[M-H]^-$ m/z Calcd for $C_{18}H_{18}ClO_5$: 349.0843. Found: 349.0847.



3o

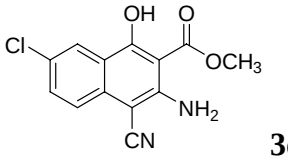
1-Ethyl 3-methyl 6-chloro-4-hydroxy-2-propylnaphthalene-1,3-dicarboxylate (3o). Eluent: petroleum ether/ethyl acetate (10:1). Yield 130 mg (74%). White solid,

mp 118-120 °C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 12.70 (s, 1H), 8.38 (s, 1H), 7.55-7.51 (m, 2H), 4.50 (q, 2H, *J* = 7.2 Hz), 4.03 (s, 3H), 2.99-2.89 (m, 2H), 1.68-1.53 (m, 2H), 1.44 (t, 3H, *J* = 7.2 Hz), 0.98 (t, 3H, *J* = 7.2 Hz). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 172.5, 169.7, 162.0, 137.4, 131.9, 131.3, 130.9, 126.0, 124.6, 124.5, 123.6, 106.3, 61.7, 52.9, 35.9, 25.3, 14.7, 14.4. HR-MS $[M-H]^-$ m/z Calcd for $C_{18}H_{18}ClO_5$: 349.0843. Found: 349.0843.



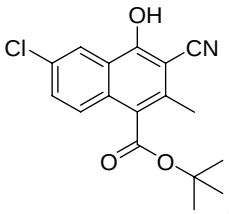
3p

Methyl 7-chloro-4-cyano-1-hydroxy-3-phenyl-2-naphthoate (3p). Eluent: petroleum ether/ethyl acetate (8:1). Yield 105 mg (62%). White solid, dp 162 °C (deccomposed point). ^{1}H NMR ($CDCl_3$, 300 MHz) δ 12.90 (s, 1H), 8.48 (s, 1H), 8.14 (d, 1H, *J* = 8.9 Hz), 7.81-7.71 (m, 1H), 7.51-7.42 (m, 3H), 7.35-7.28 (m, 2H), 3.50 (s, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 171.2, 163.4, 147.5, 139.3, 133.8, 133.0, 132.8, 128.5, 128.3, 128.1, 127.2, 124.9, 123.9, 116.6, 107.4, 103.3, 52.7. HR-MS $[M-H]^-$ m/z Calcd for $C_{19}H_{11}ClNO_3$: 336.0428. Found: 336.0429.



3q

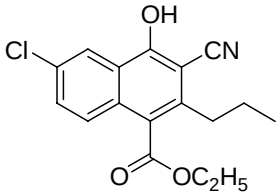
Methyl 3-amino-7-chloro-4-cyano-1-hydroxy-2-naphthoate (3q). Eluent: petroleum ether/ethyl acetate (5:1). Yield 94 mg (68%). Yellow solid, mp 231-233 °C. ^{1}H NMR (DMSO-d_6, 300 MHz) δ 12.68 (s, 1H), 8.04 (d, 1H, *J* = 5.2 Hz), 7.79-7.49 (m, 2H), 7.00 (s, 2H), 3.99 (s, 3H). ^{13}C NMR (DMSO-d_6, 75 MHz) δ 169.3, 162.9, 151.6, 134.4, 132.5, 127.1, 124.0, 123.1, 118.5, 117.1, 98.7, 78.4, 53.4. HR-MS $[M-H]^-$ m/z Calcd for $C_{13}H_8ClN_2O_3$: 275.0223. Found: 275.0221.



3r

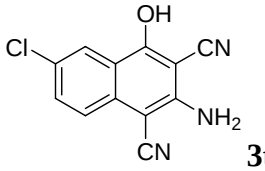
***tert*-Butyl 6-chloro-3-cyano-4-hydroxy-2-methyl-1-naphthoate (3r).** Eluent: ethyl

acetate and then washed with ethyl ether. Yield 92 mg (58%). White solid, dp 193 °C (deccomposed point). ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.20 (d, 1H, *J* = 2.1 Hz), 7.74 (d, 1H, *J* = 9.3 Hz), 7.59 (dd, 1H, *J* = 2.1 Hz，*J* = 9.3 Hz), 6.87 (s, 1H), 2.59 (s, 3H), 1.68 (s, 9H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 167.5, 157.2, 132.7, 132.6, 131.5, 131.0, 126.4, 126.1, 122.9, 122.3, 115.4, 96.0, 83.7, 28.4, 18.9. HR-MS $[M-H]^-$ m/z Calcd for $C_{17}H_{15}ClNO_3$: 316.0740. Found: 316.0739.



3s

Methyl 6-chloro-3-cyano-4-hydroxy-2-propyl-1-naphthoate (3s). Eluent: ethyl acetate and then washed with ethyl ether. Yield 87 mg (55%). White solid, mp 100-102 °C. ^{1}H NMR (DMSO-d_6, 300 MHz) δ 8.41 (s, 1H), 7.82-7.69 (m, 2H), 4.45 (q, 2H, *J* = 6.9 Hz), 2.81-2.71 (m, 2H), 1.74-1.57 (m, 2H), 1.36 (t, 3H, *J* = 6.9 Hz), 0.97 (t, 3H, *J* = 7.2 Hz). ^{13}C NMR (DMSO-d_6, 150 MHz) δ 167.5, 160.2, 138.9, 130.9, 130.6, 127.1, 124.1, 122.2, 116.1, 96.2, 61.5, 34.6, 23.7, 14.0, 13.9. HR-MS $[M-H]^-$ m/z Calcd for $C_{17}H_{15}ClNO_3$: 316.0740. Found: 316.0742.



3t

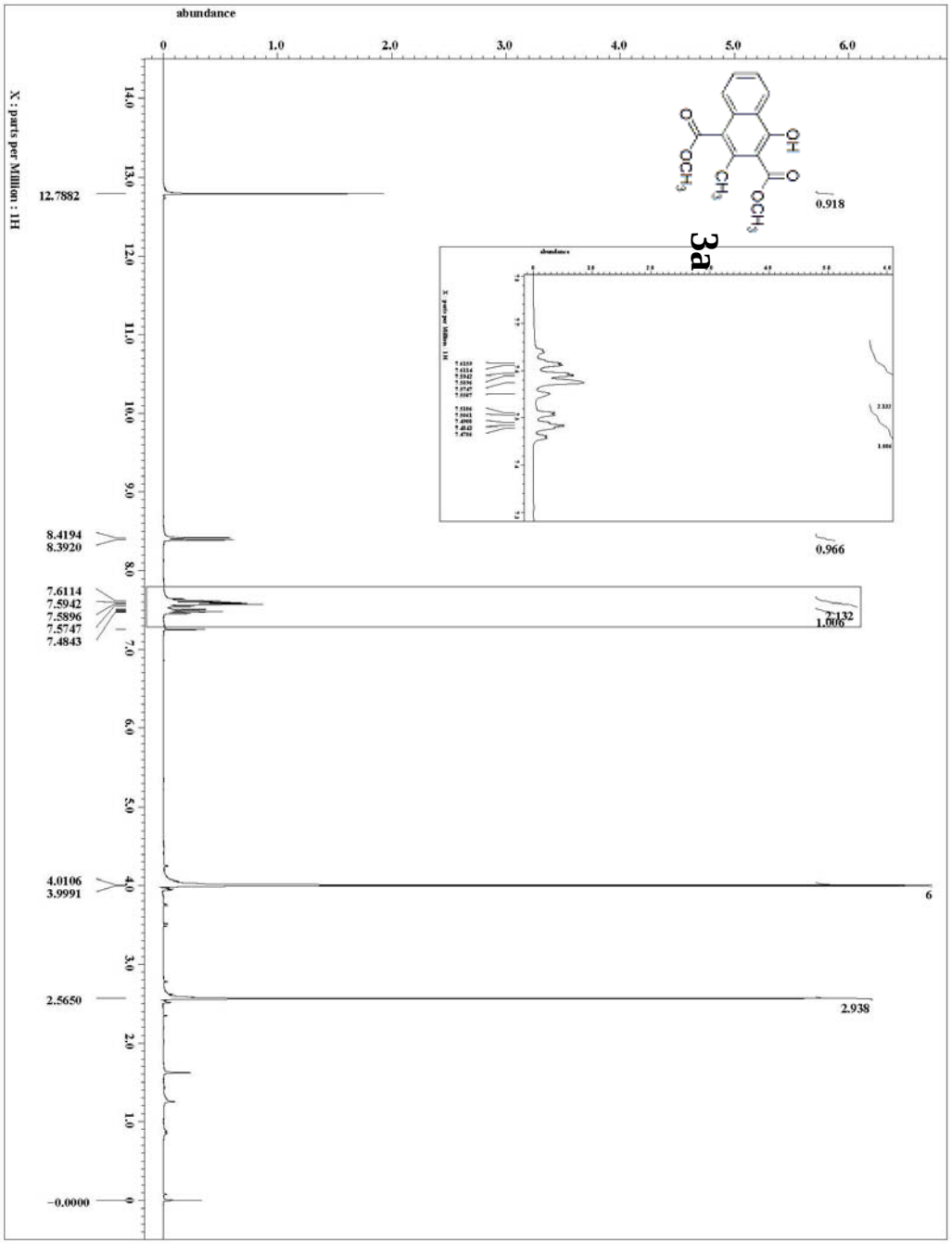
2-Amino-6-chloro-4-hydroxynaphthalene-1,3-dicarbonitrile (3t). Eluent: ethyl acetate/methanol (20:1) and then recrystalization from ethyl acetate/hexane. Yield 94 mg (77%). White solid, mp >300 °C. ^{1}H NMR (DMSO-d_6, 300 MHz) δ 7.95 (s, 1H), 7.48-7.29 (m, 2H), 5.62 (s, 1H). ^{13}C NMR (DMSO-d_6, 75 MHz) δ 174.5, 156.0, 135.4, 130.2, 126.8, 125.2, 124.9, 124.7, 120.1, 120.0, 82.0, 68.1. HR-MS $[M-H]^-$ m/z Calcd for $C_{12}H_5ClN_3O$: 242.0121. Found: 242.0118.

References

1 L. F. Tietze, T. Redert, H. P. Bell, S. Hellkamp, L. M. Levy, *Chem. Eur. J.,* 2008, **14**, 2527 – 2535.

2 W. Yu, Y. Du, K. Zhao, *Org. Lett*., 2009, **11**, 2417-2420.

3 Y. Matsubara, M. Morita, S. Takekuma, H. Yamamoto, T.Nozoe, *Nippon Kagaku Kaishi*, 1990, 67-71.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7.5747
7.4843
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2.5650
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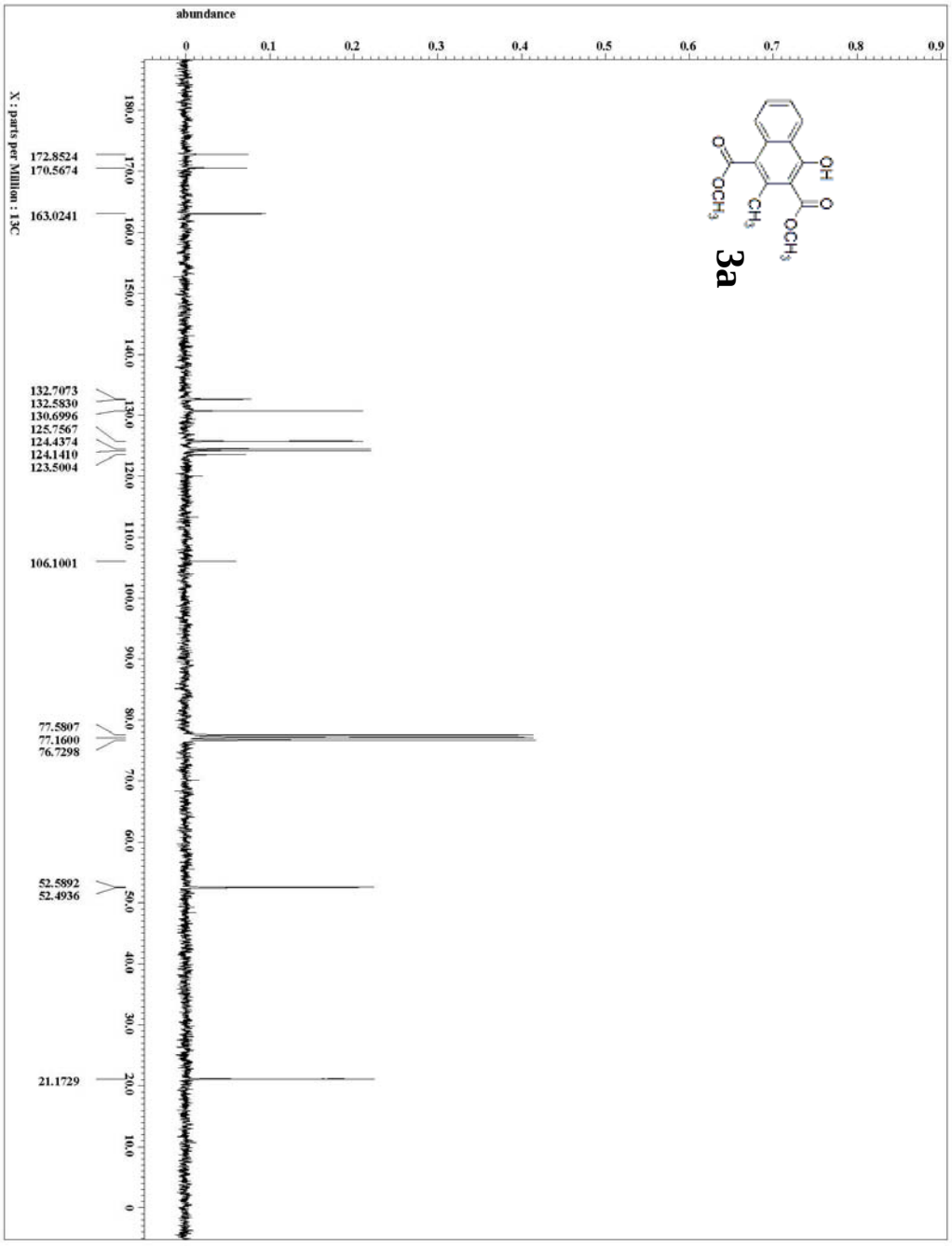
0.966
2.132
1.006
6
2.938
3a


abundance
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124.1410
123.5004
106.1001
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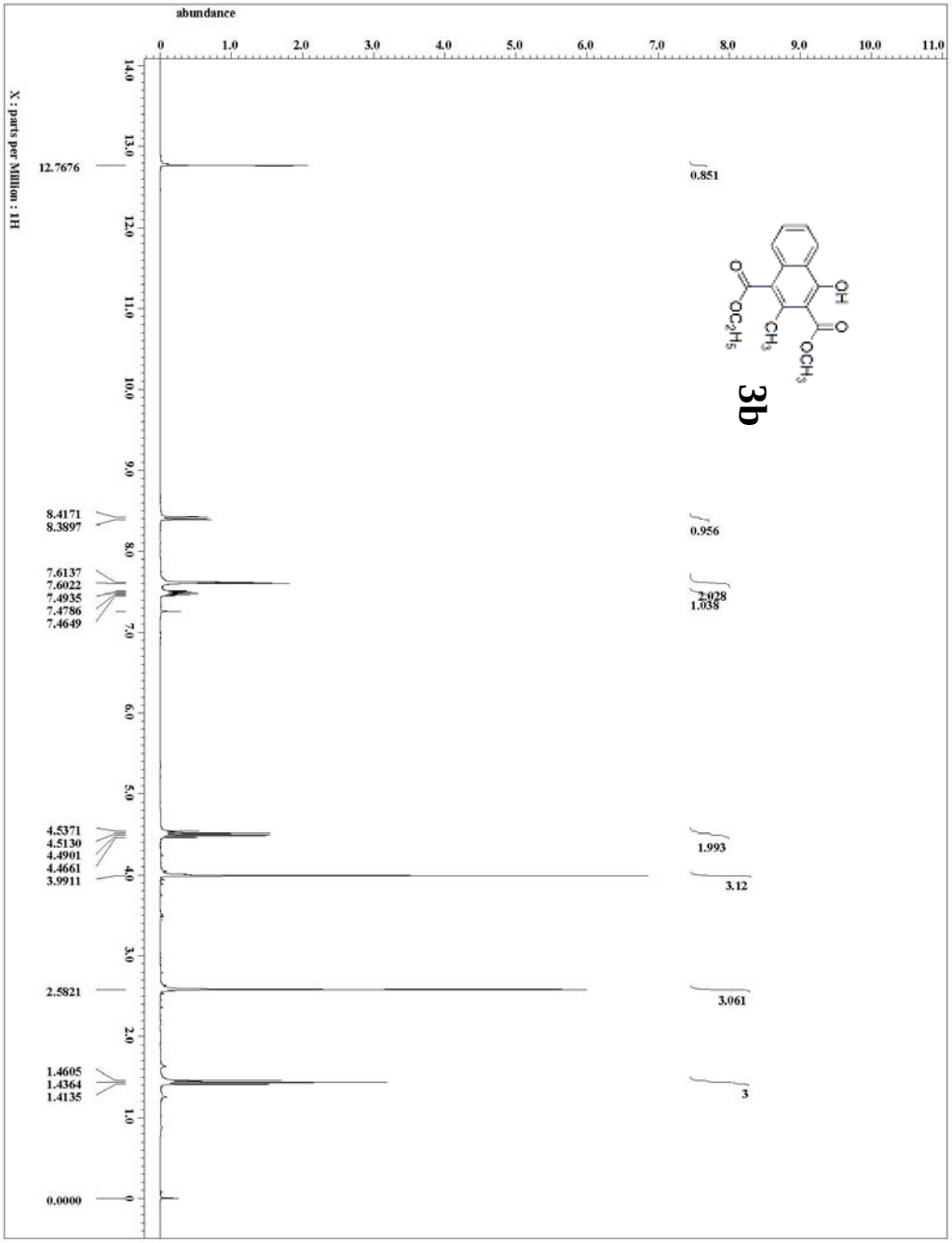
CH3
OCH3
3a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7.4649
4.5371
4.5130
4.4901
4.4661
3.9911
2.5821
1.4605
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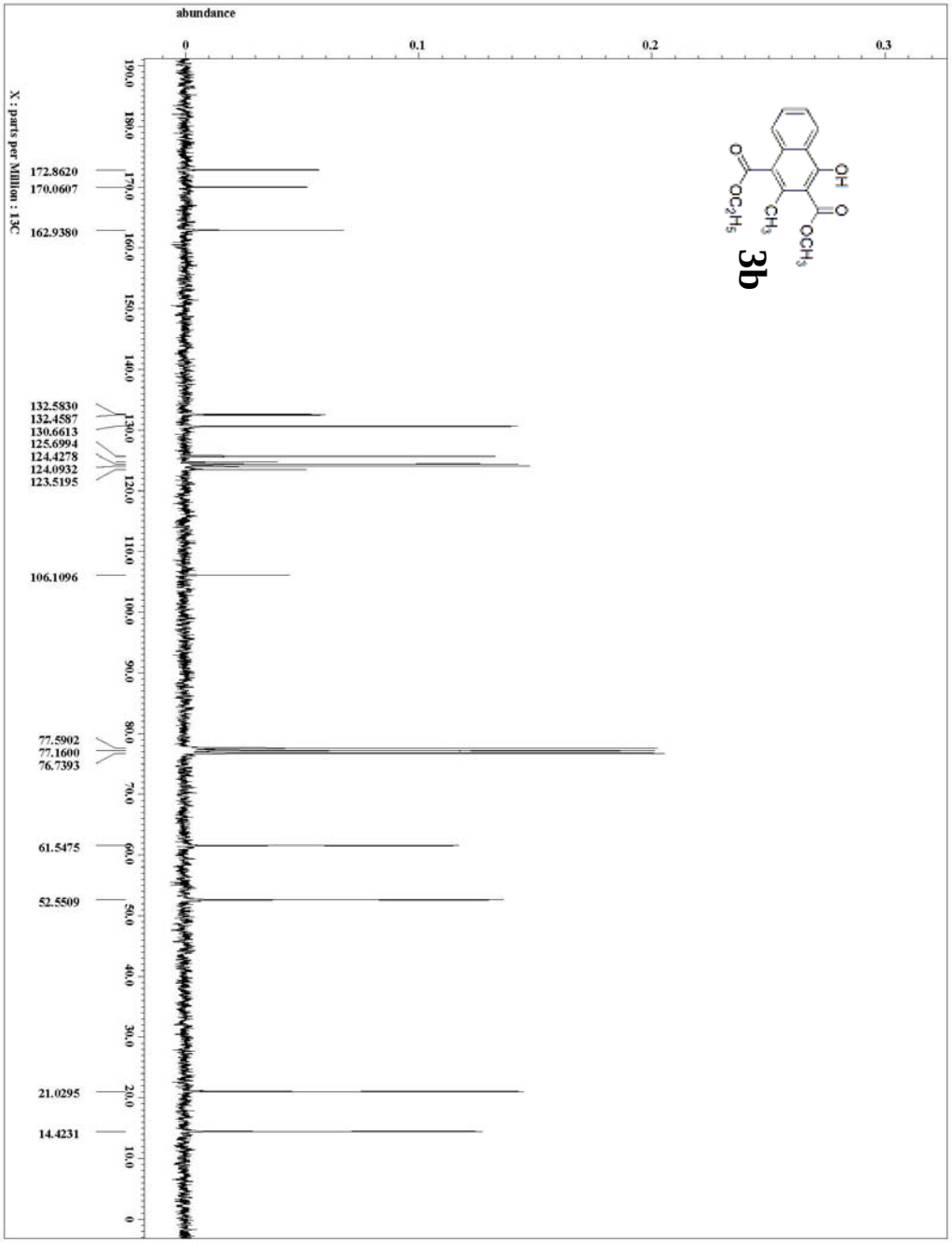
1.038
1.993
3.12
3.061
3
3b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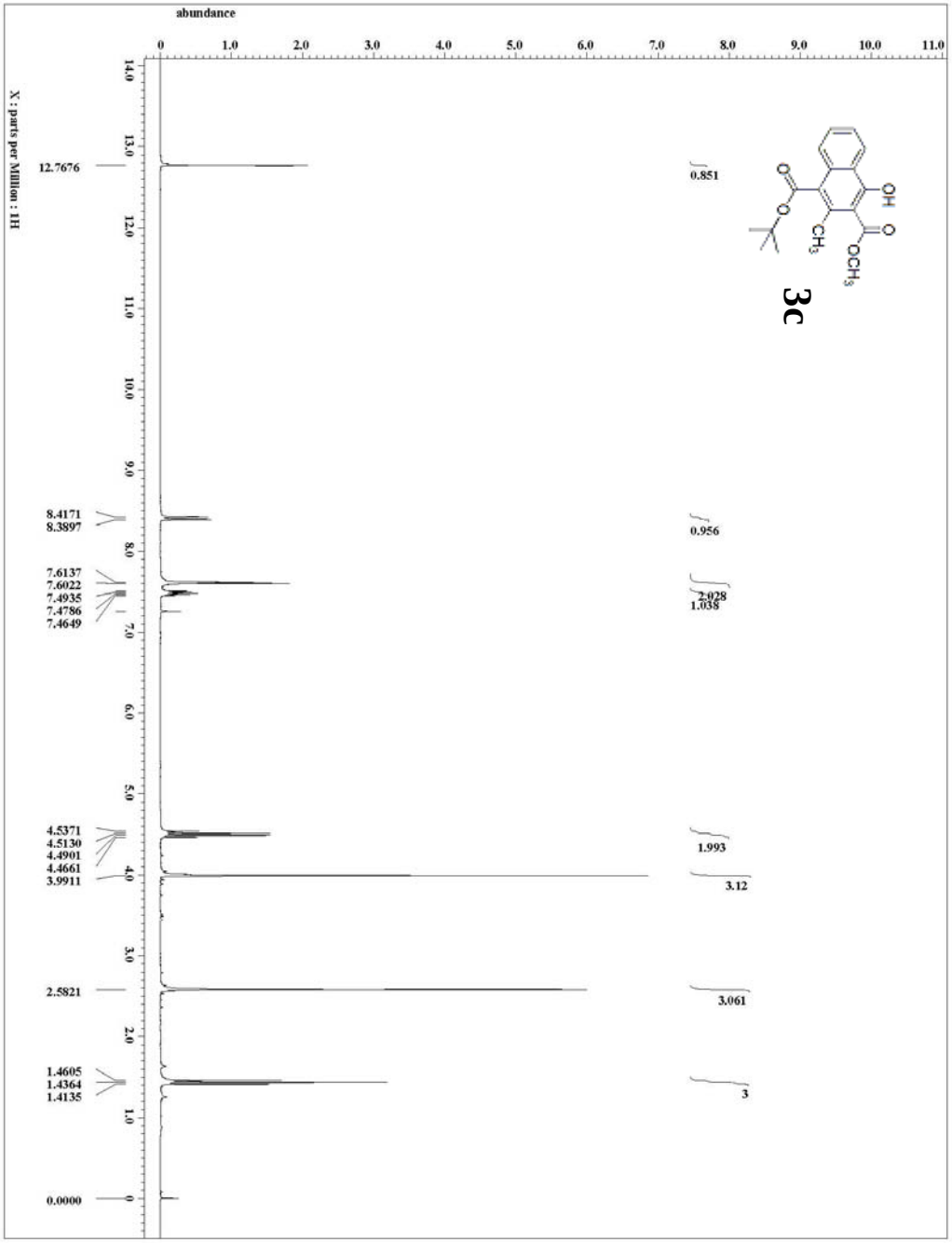
CH3
OCH3
3b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4.5371
4.5130
4.4901
4.4661
3.9911
2.5821
1.4605
1.4364
1.4135
0.0000
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1.993
3.12
3.061
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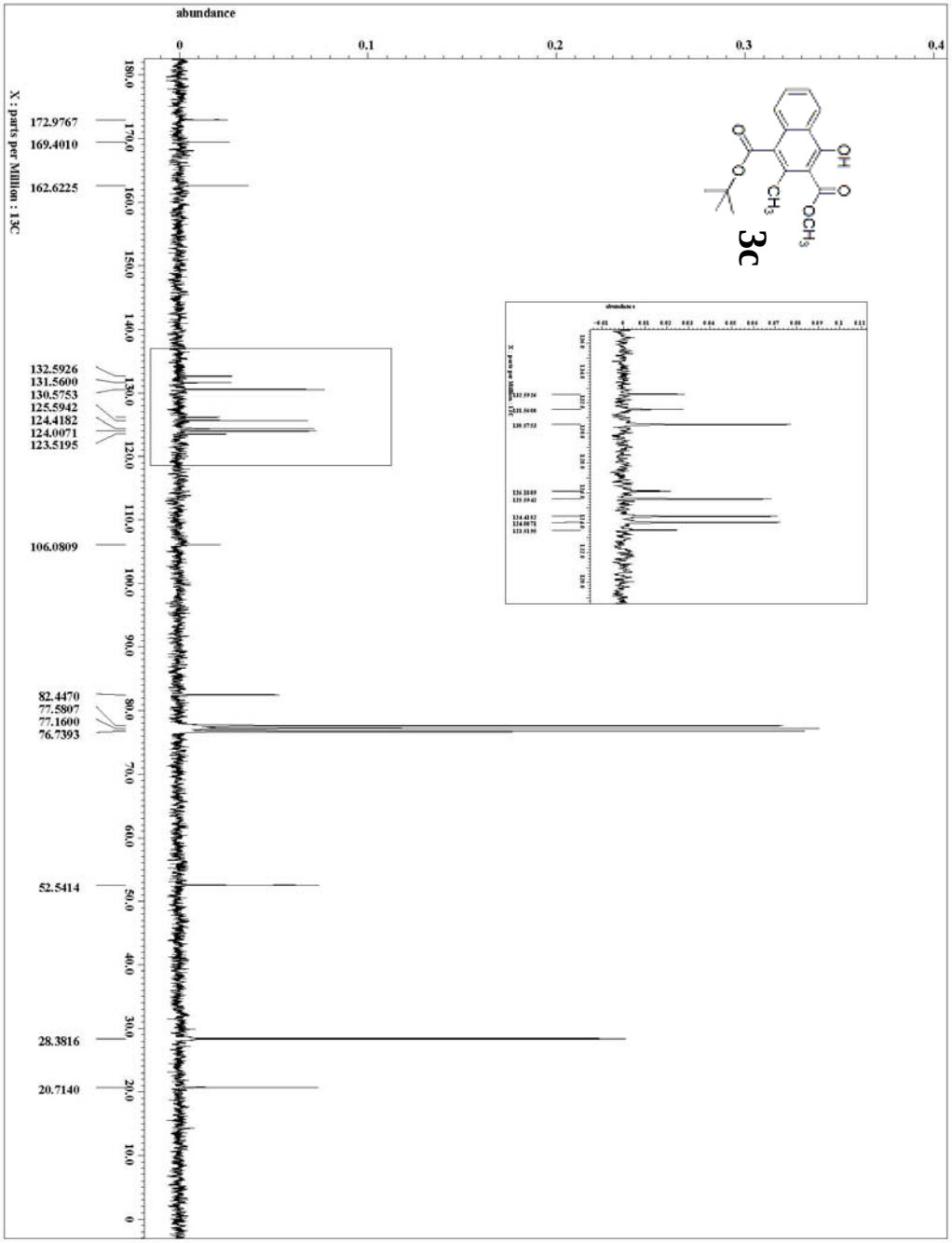
O
O
CH3
O
OCH3
3c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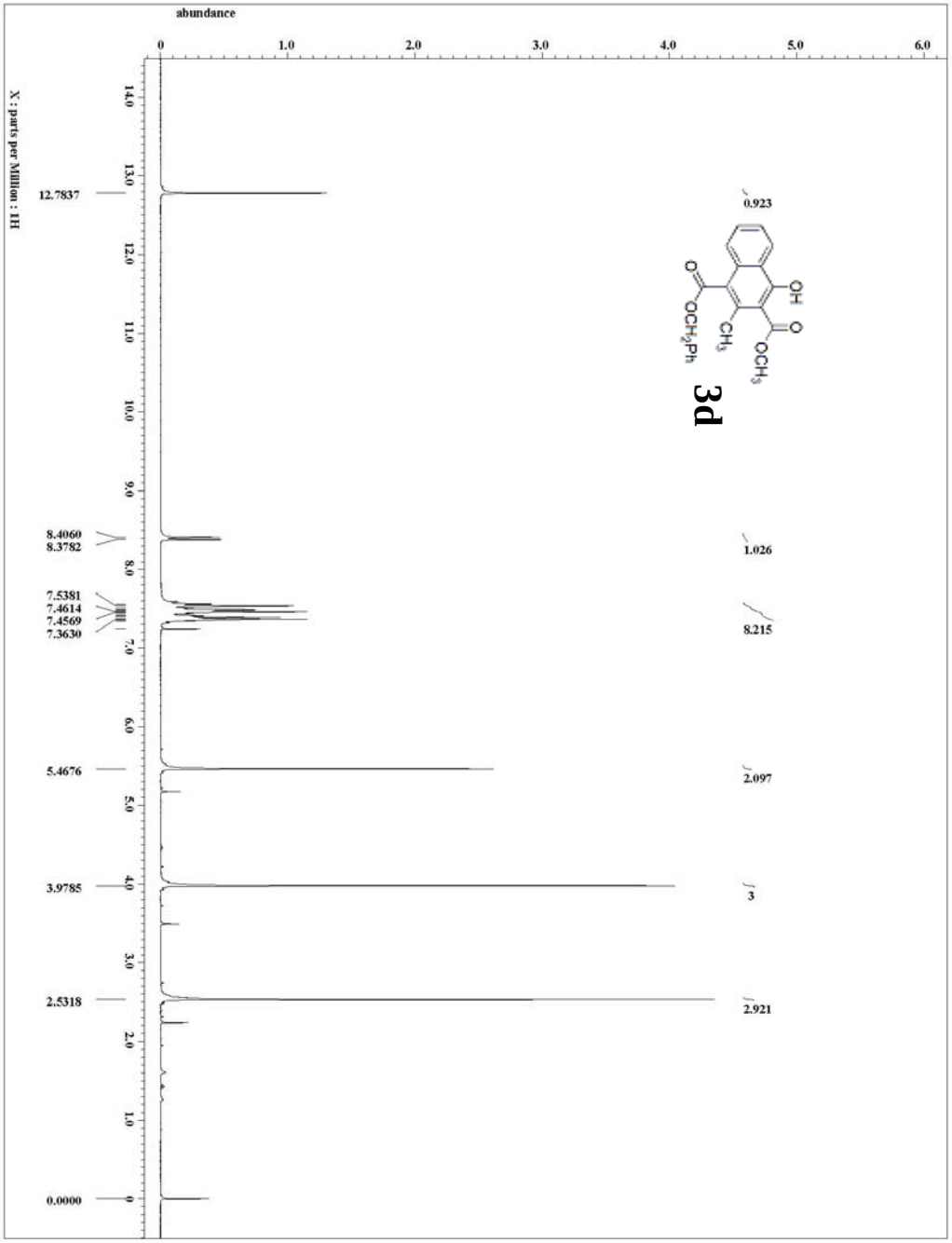
3c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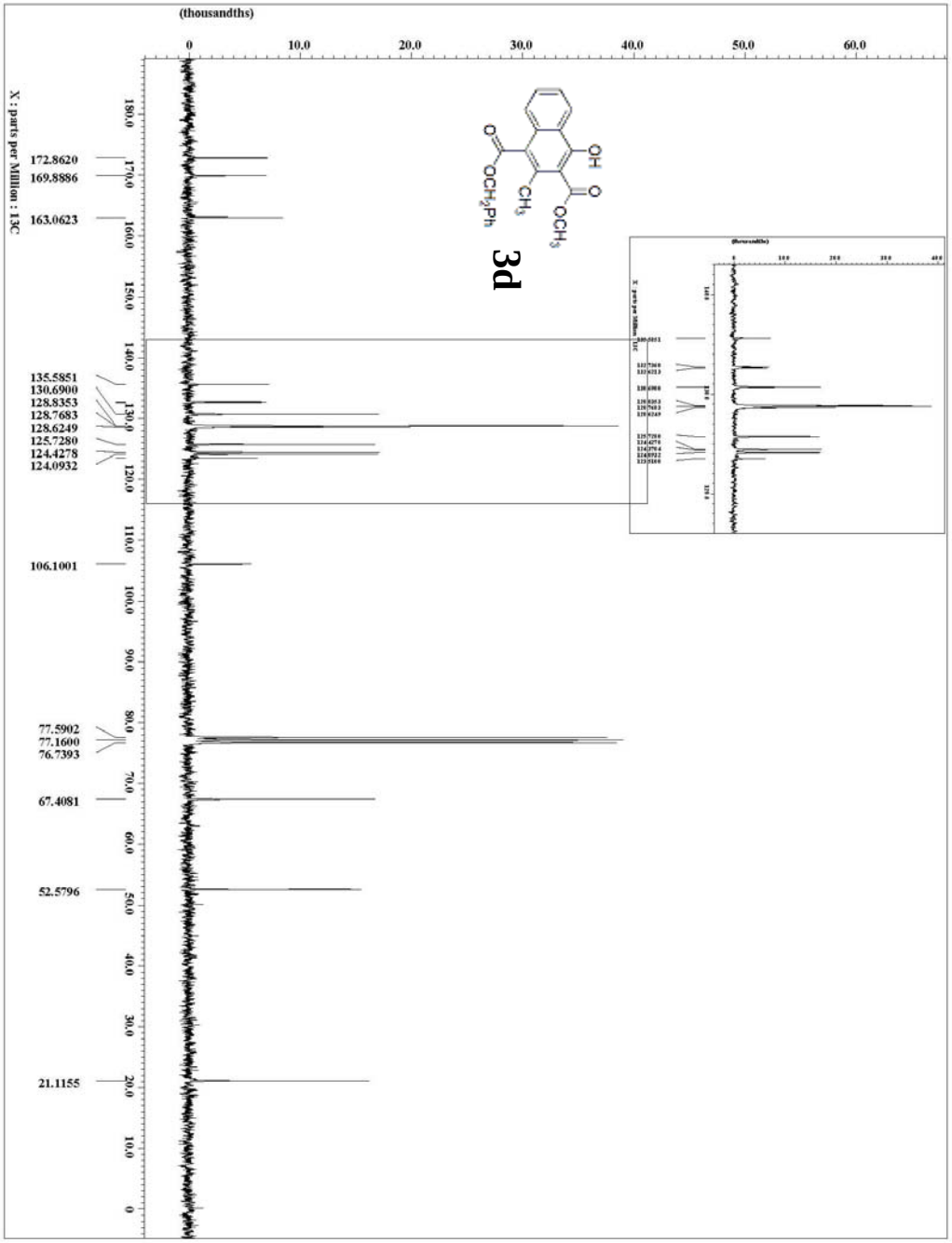
3d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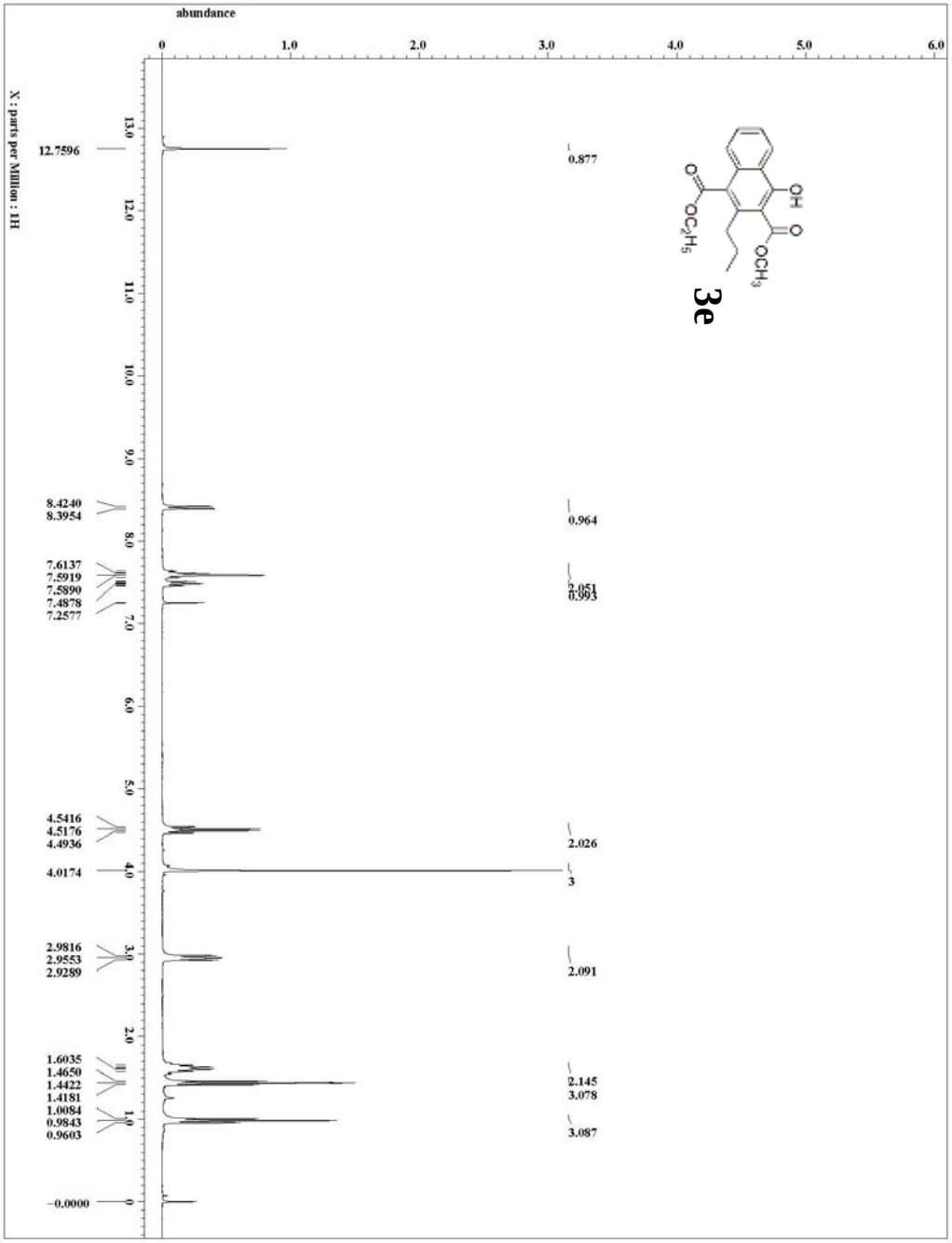
3d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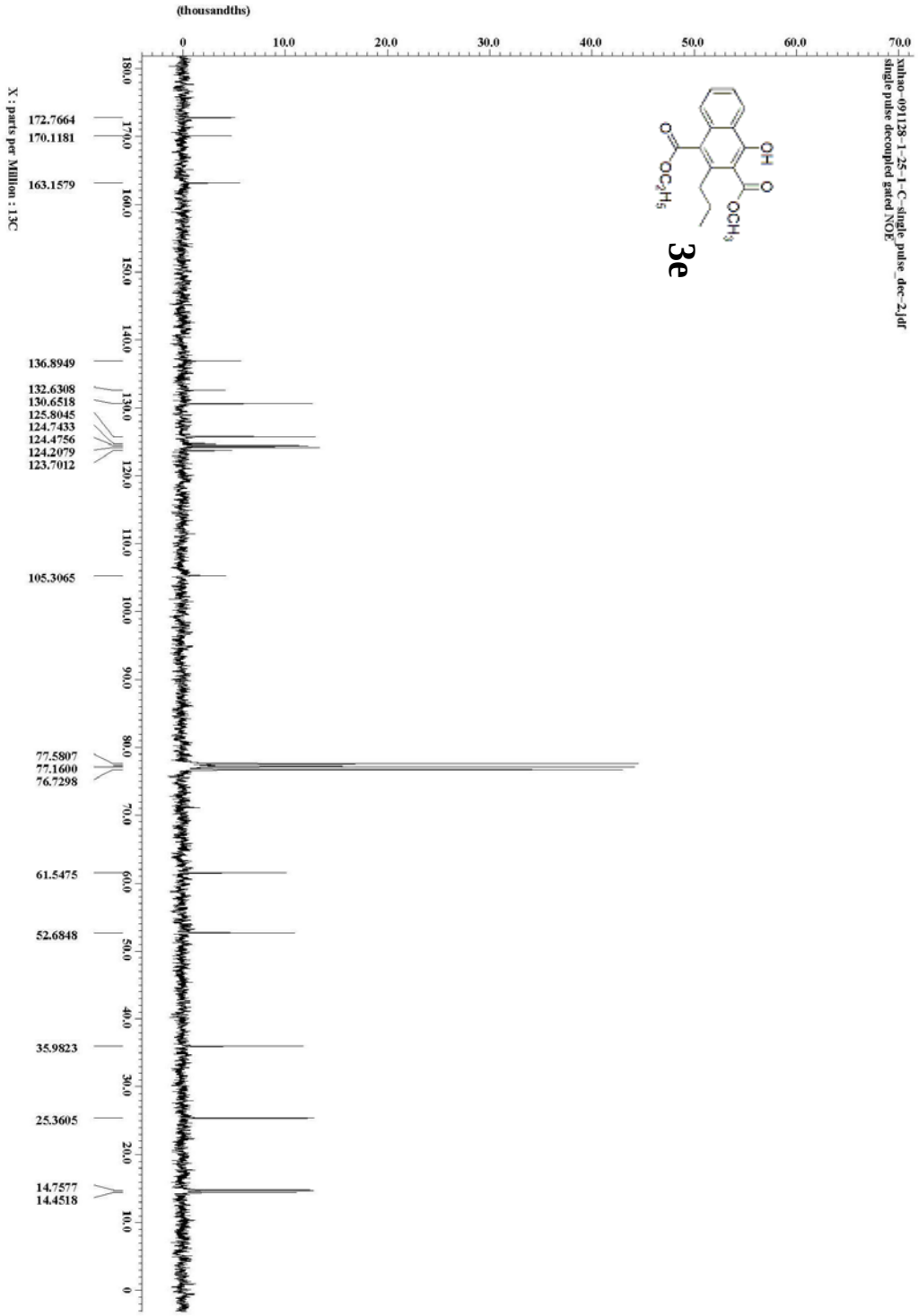
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single pulse decoupled gated NOE
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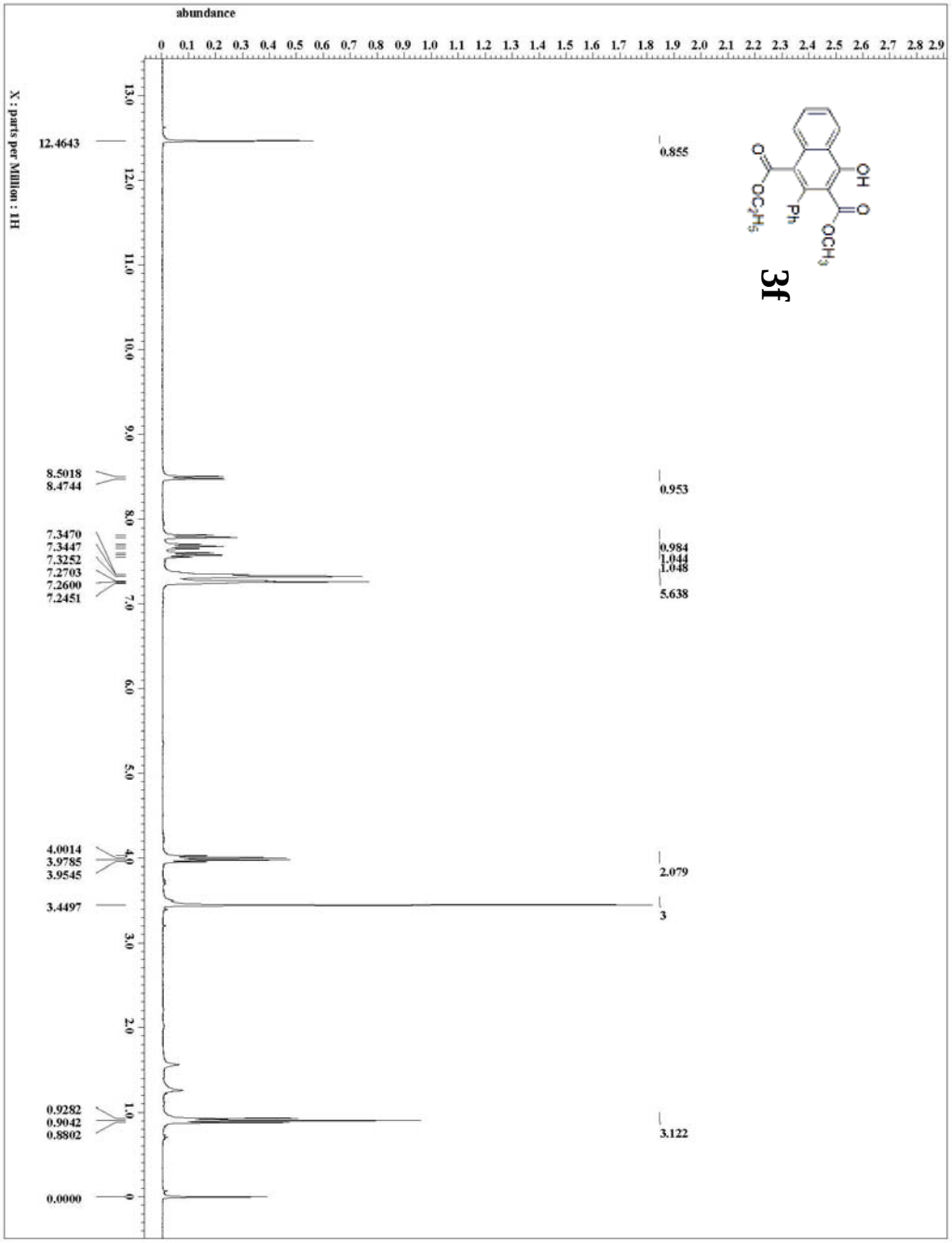
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7.2451
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3.9545
3.4497
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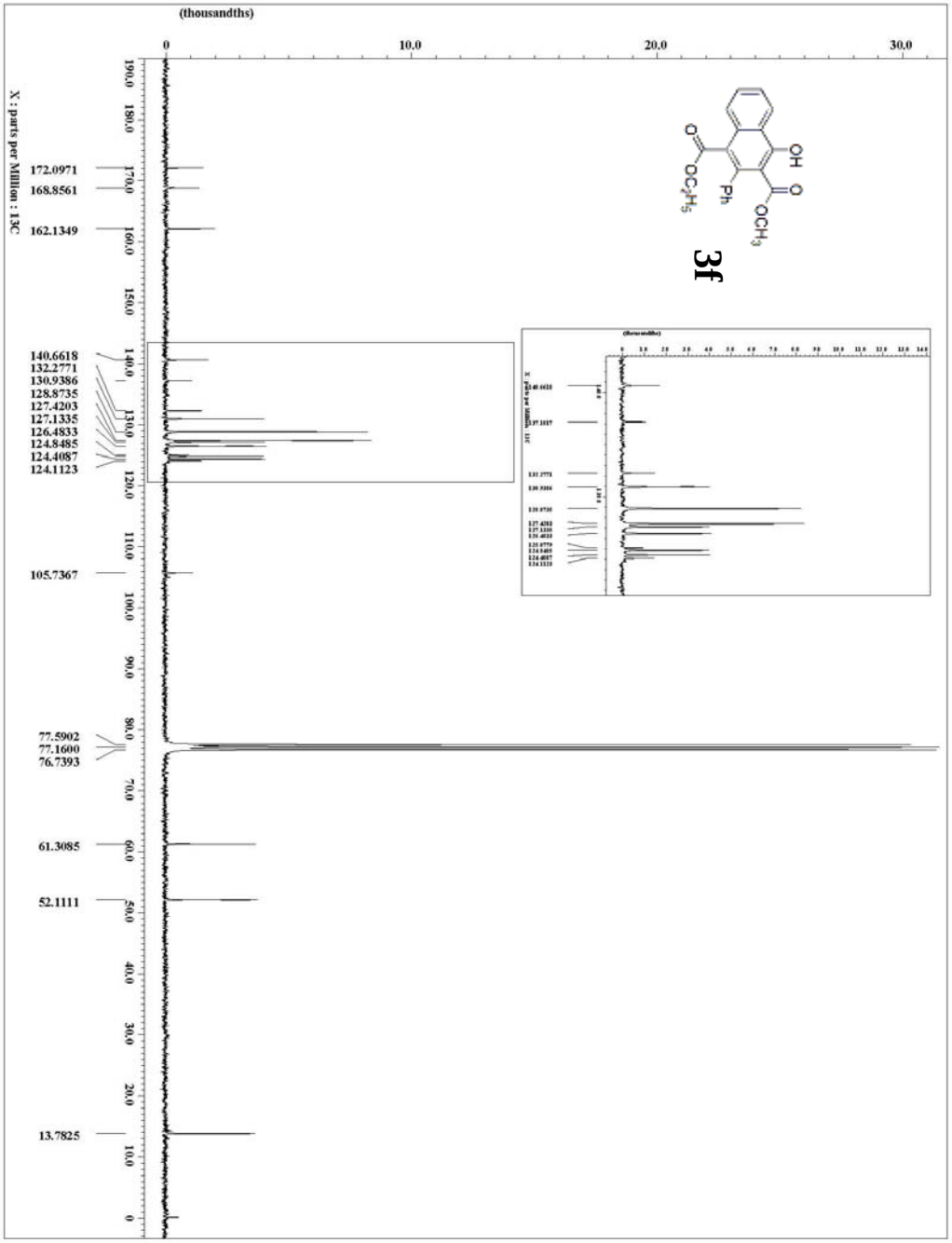
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Ph
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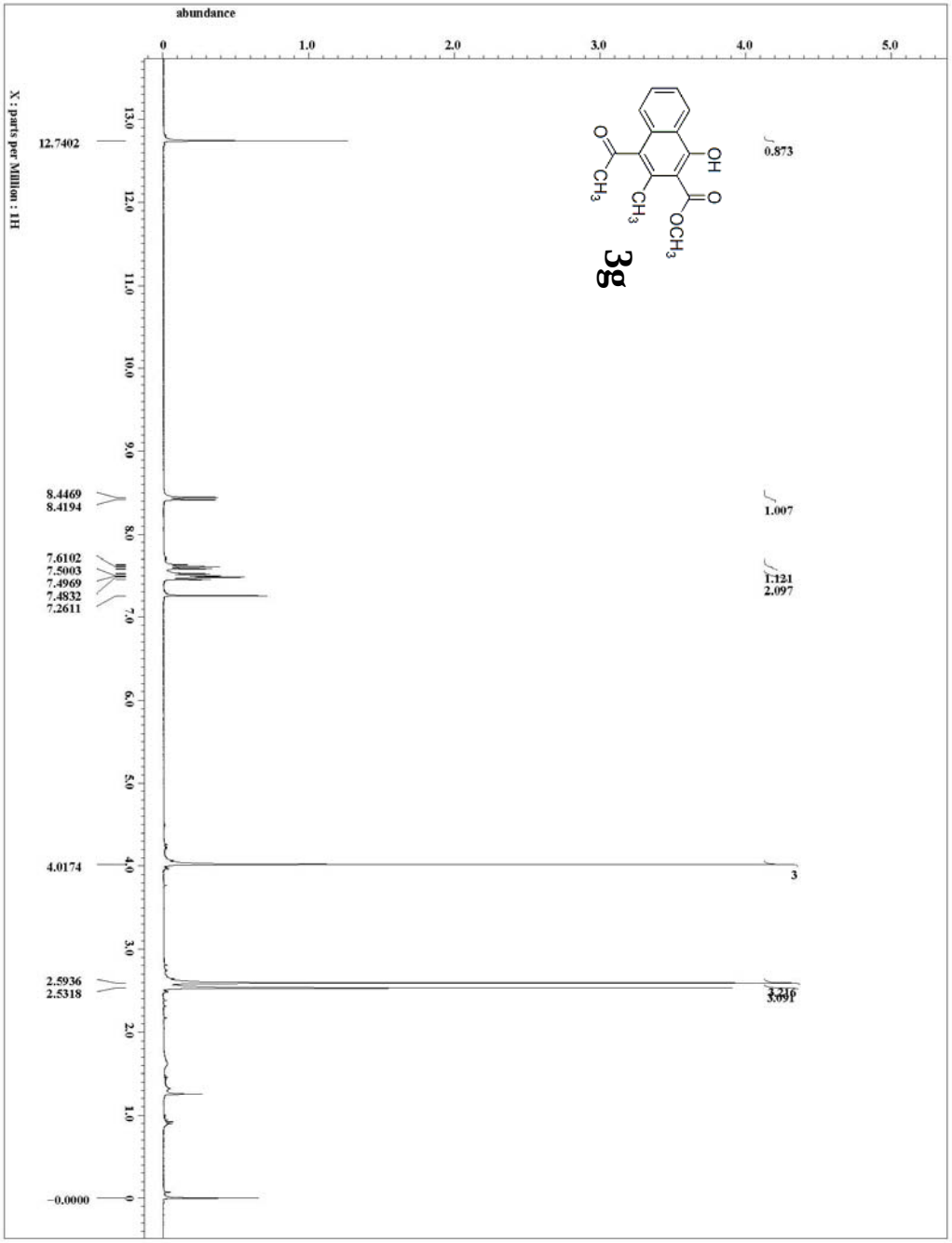
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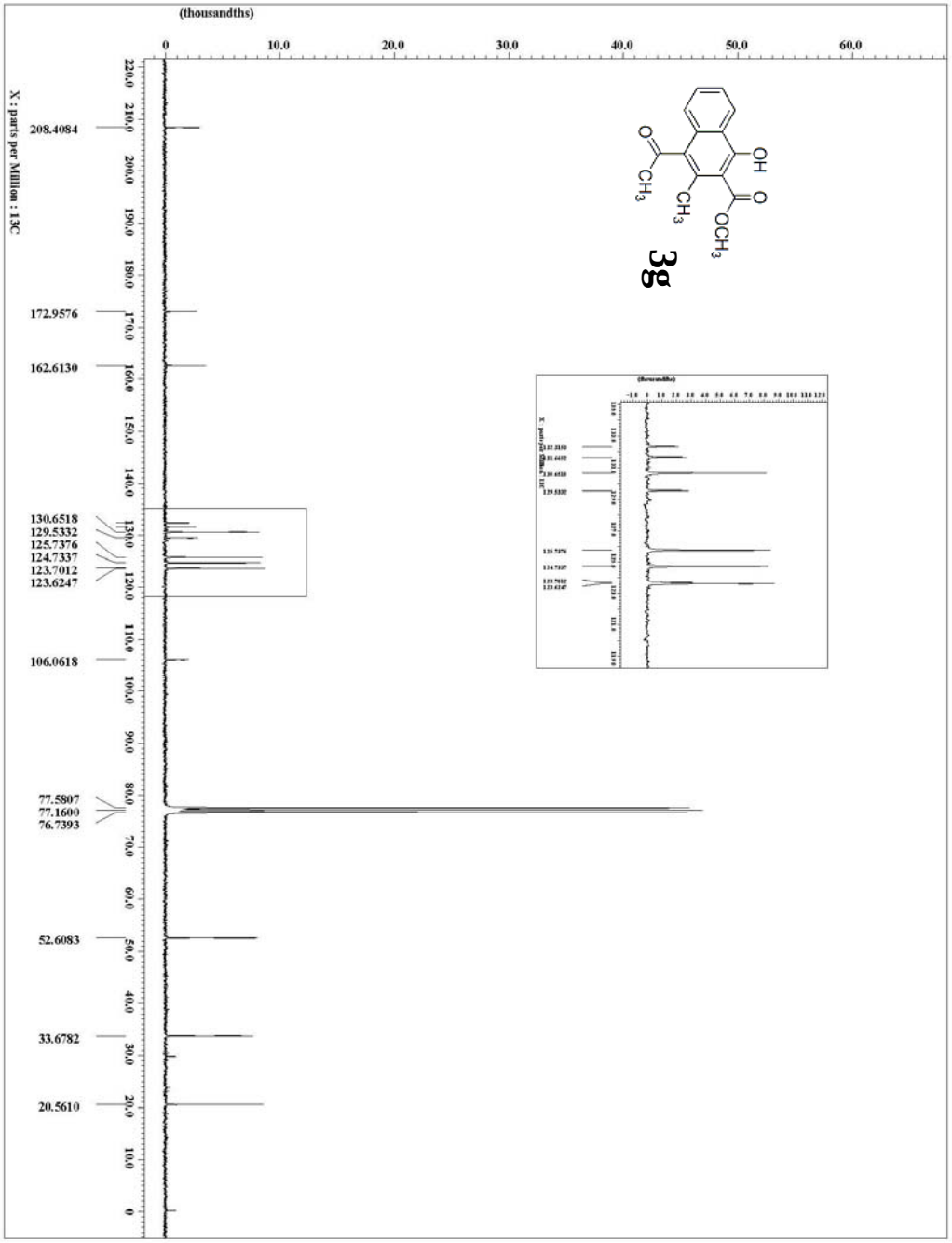
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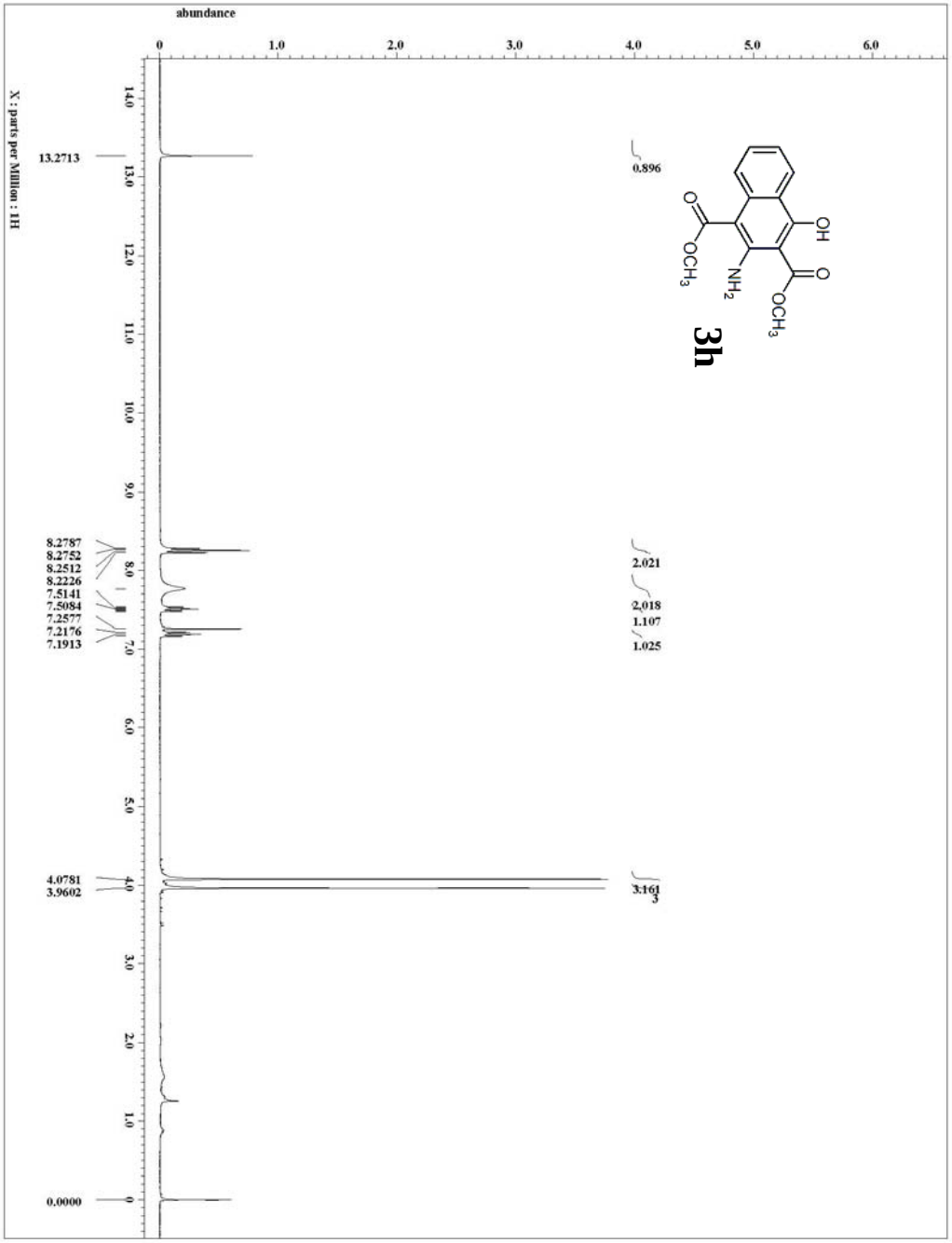
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NH2
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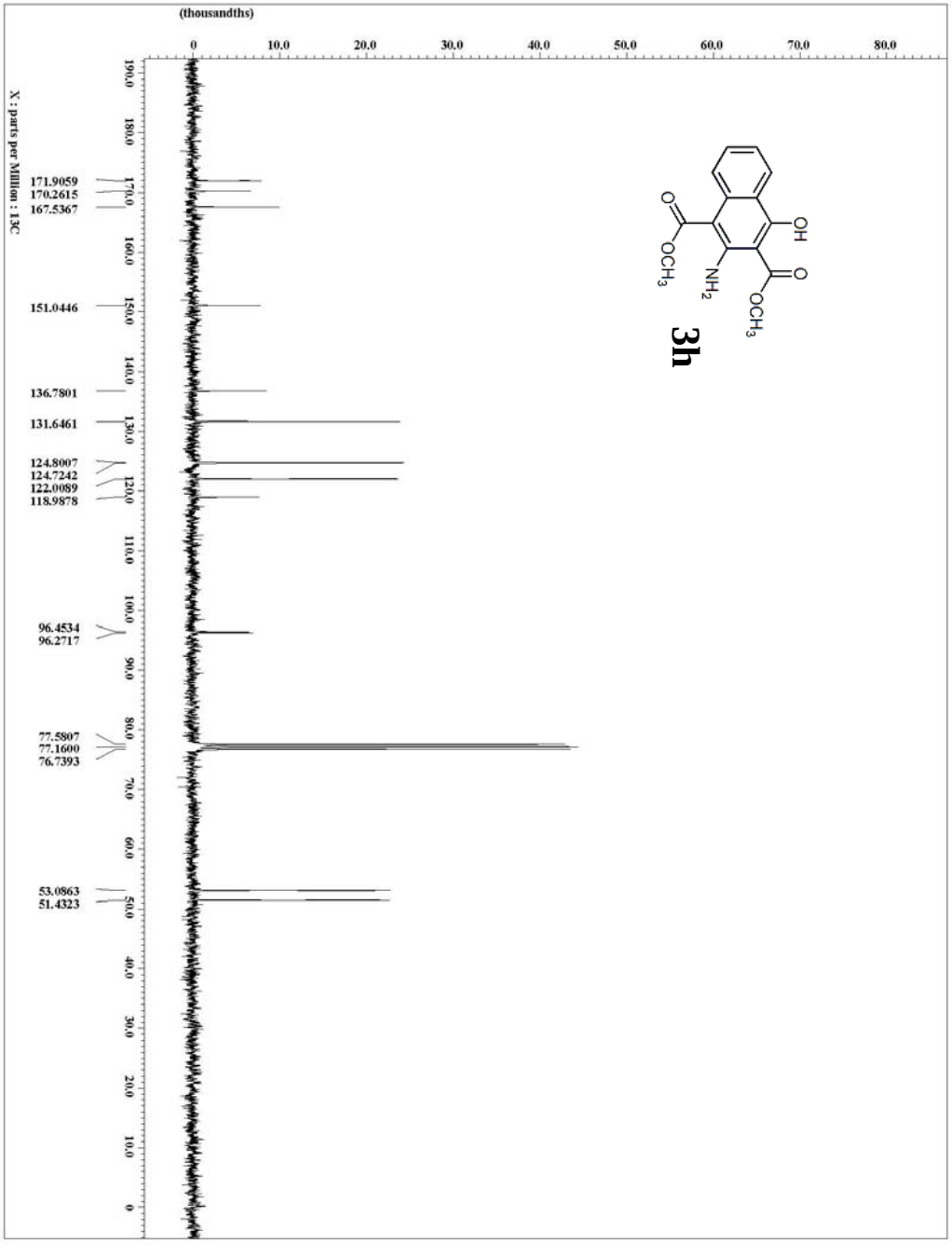
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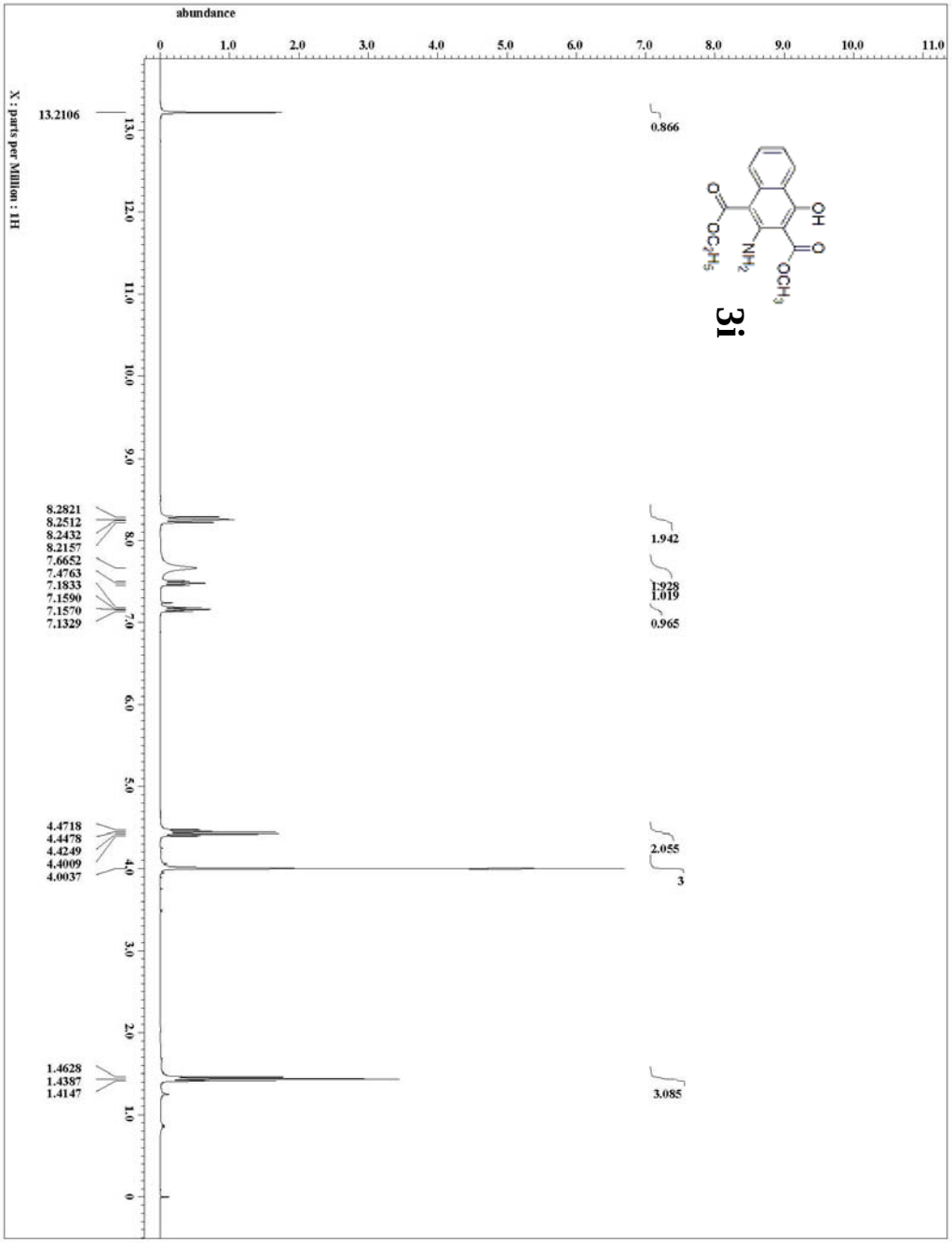
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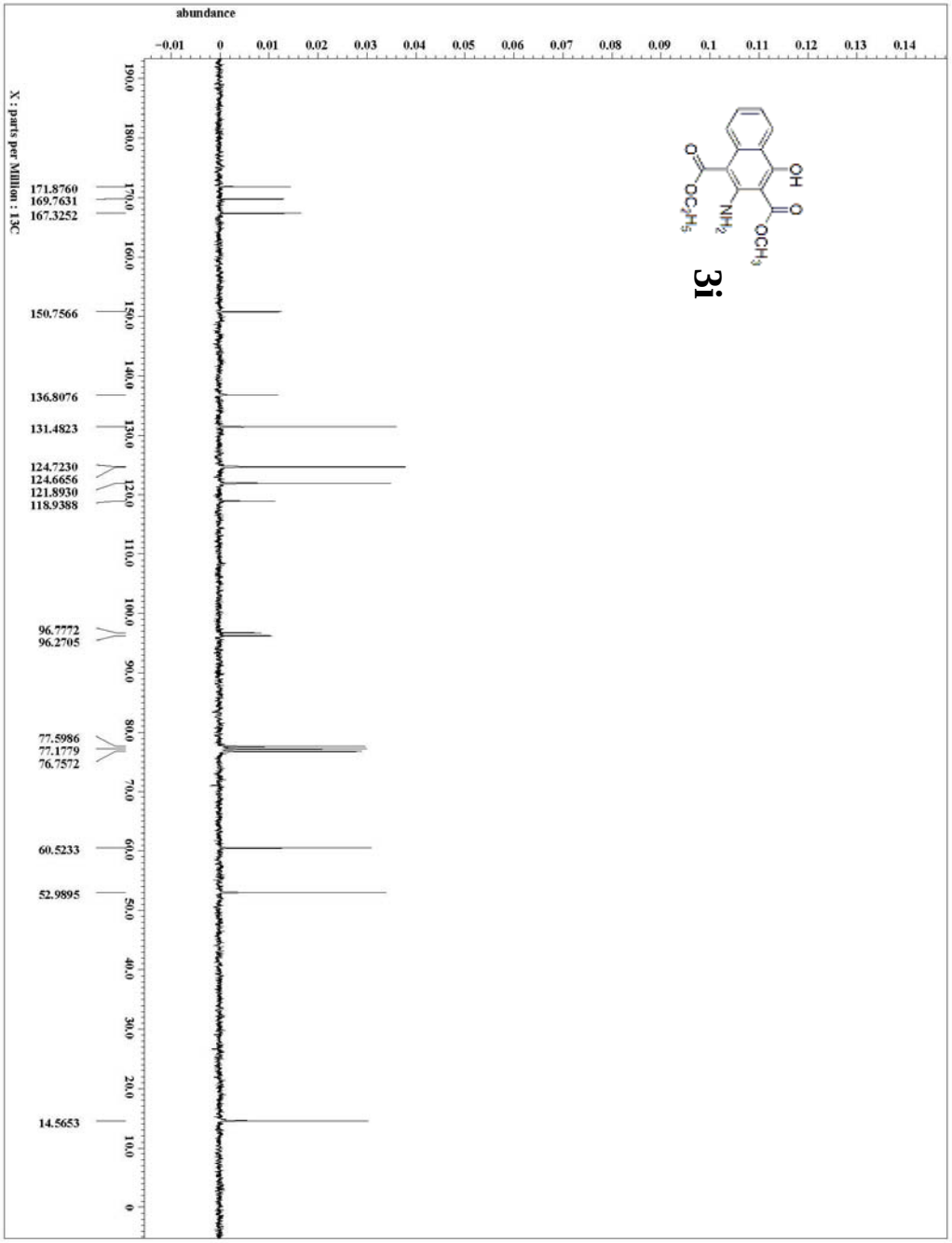
3i.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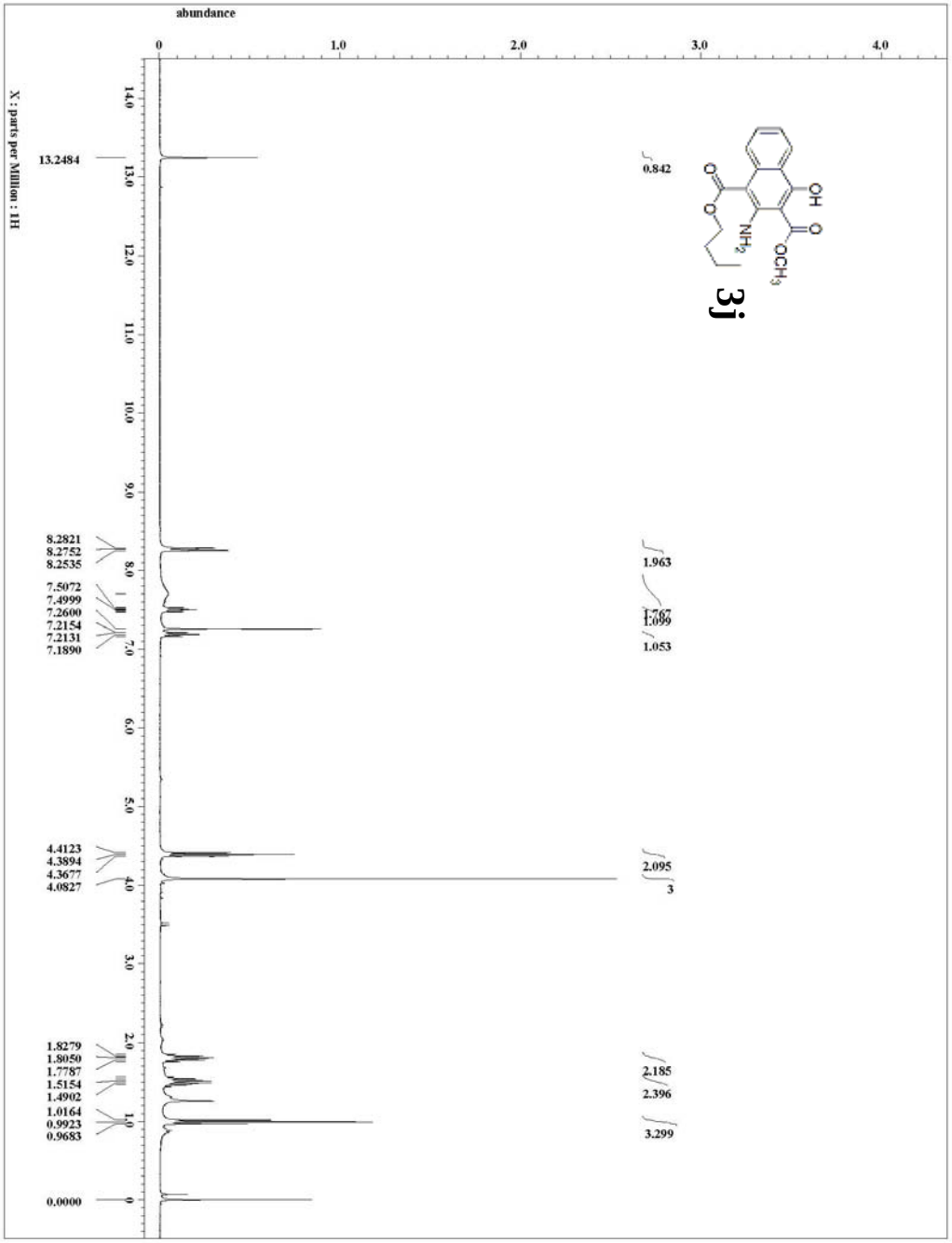
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7.1890
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4.3677
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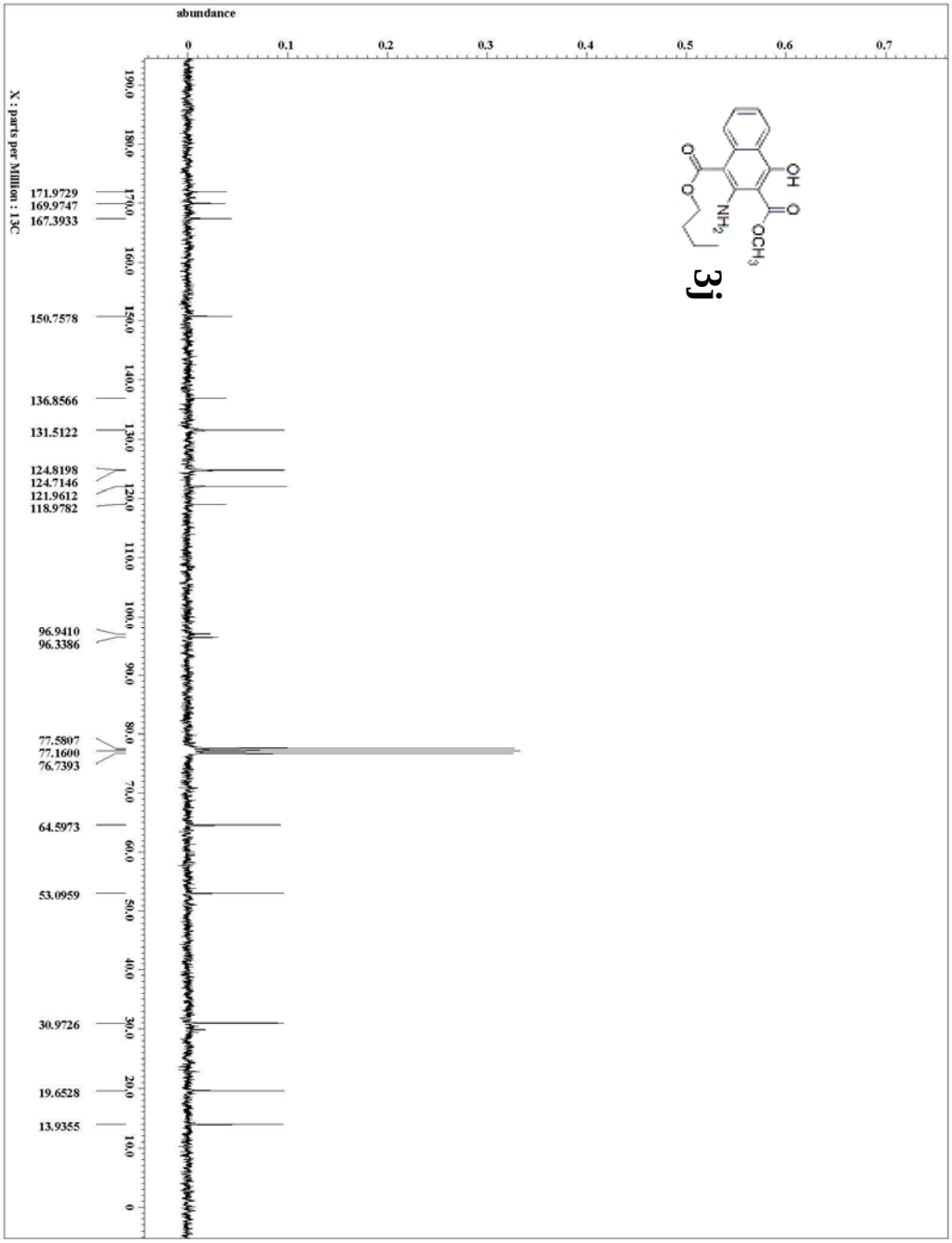
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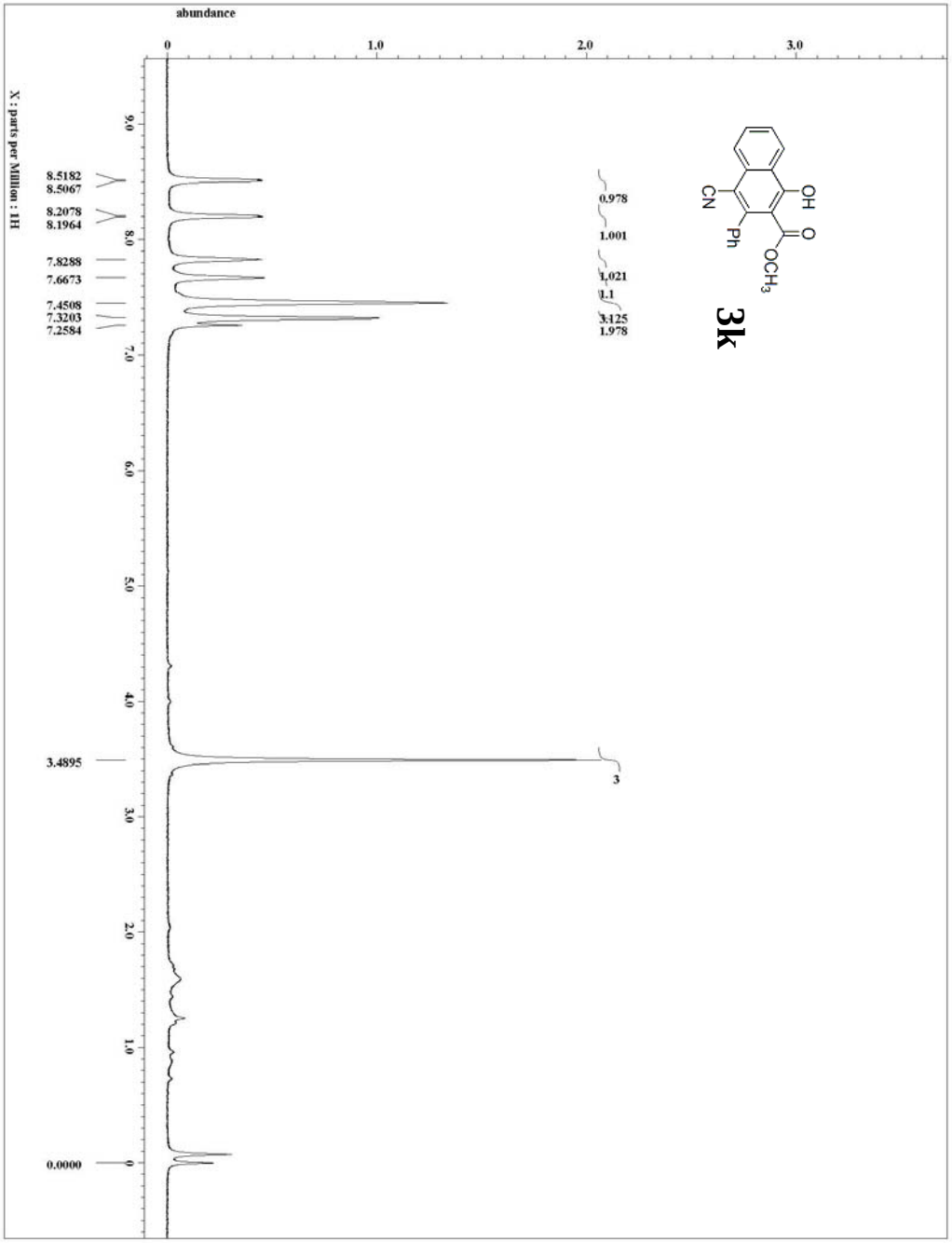
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X : parts per Million : 1H
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Ph
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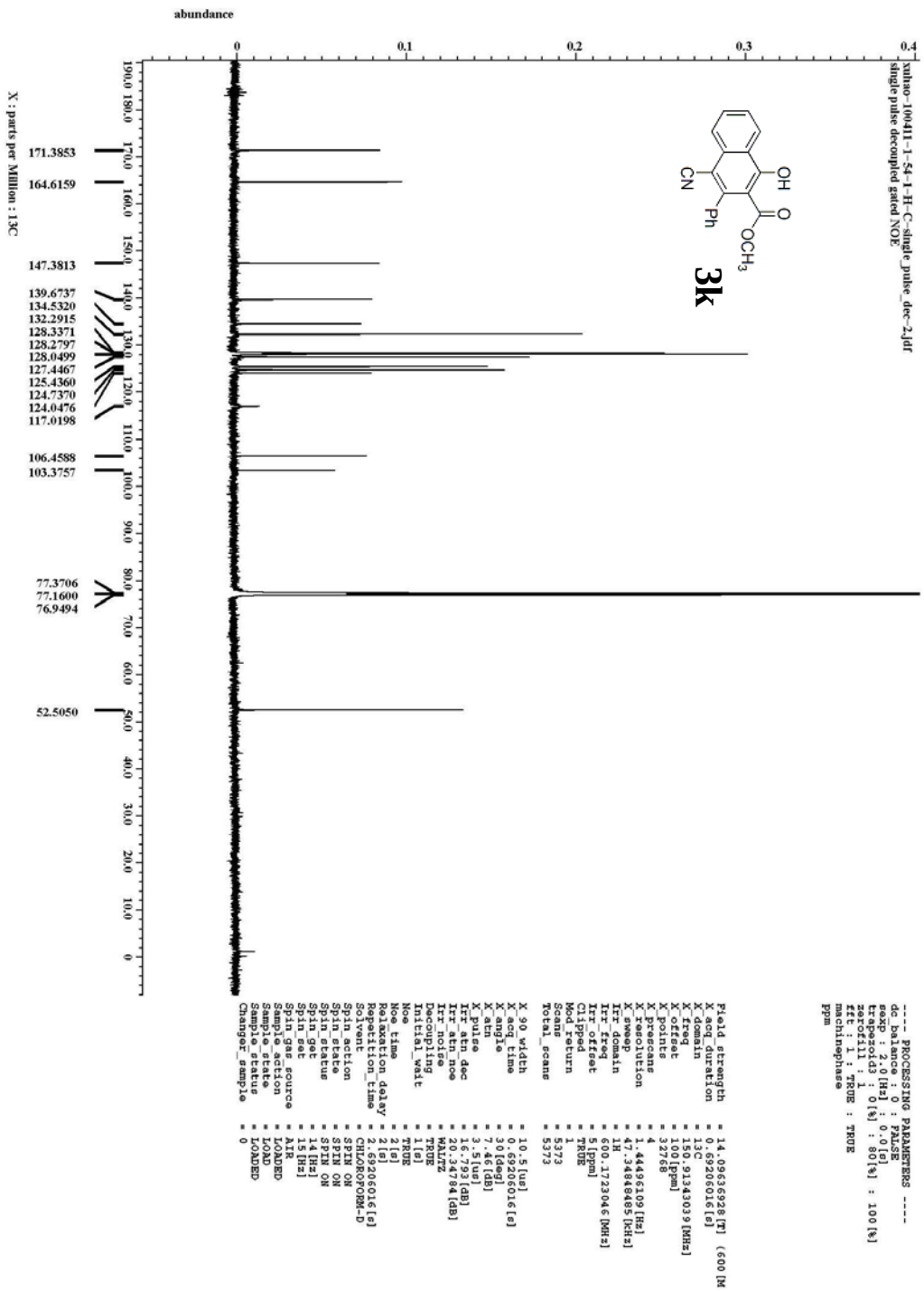
abundance
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single pulse decoupled gated NOE
3k
OH
O
OCH3
CN
Ph
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164.6159
147.3813
139.6737
134.5320
132.2915
128.3371
128.2797
128.0499
127.4467
125.4360
124.7370
124.0476
117.0198
106.4588
103.3757
77.3706
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76.9494
52.5050
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trapezoid : 0 [%] : 80 [%] : 100 [%]
zerofill : 1 : TRUE : TRUE
fft : 1 : TRUE : TRUE
machinephase
ppm
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X_domain = 13C
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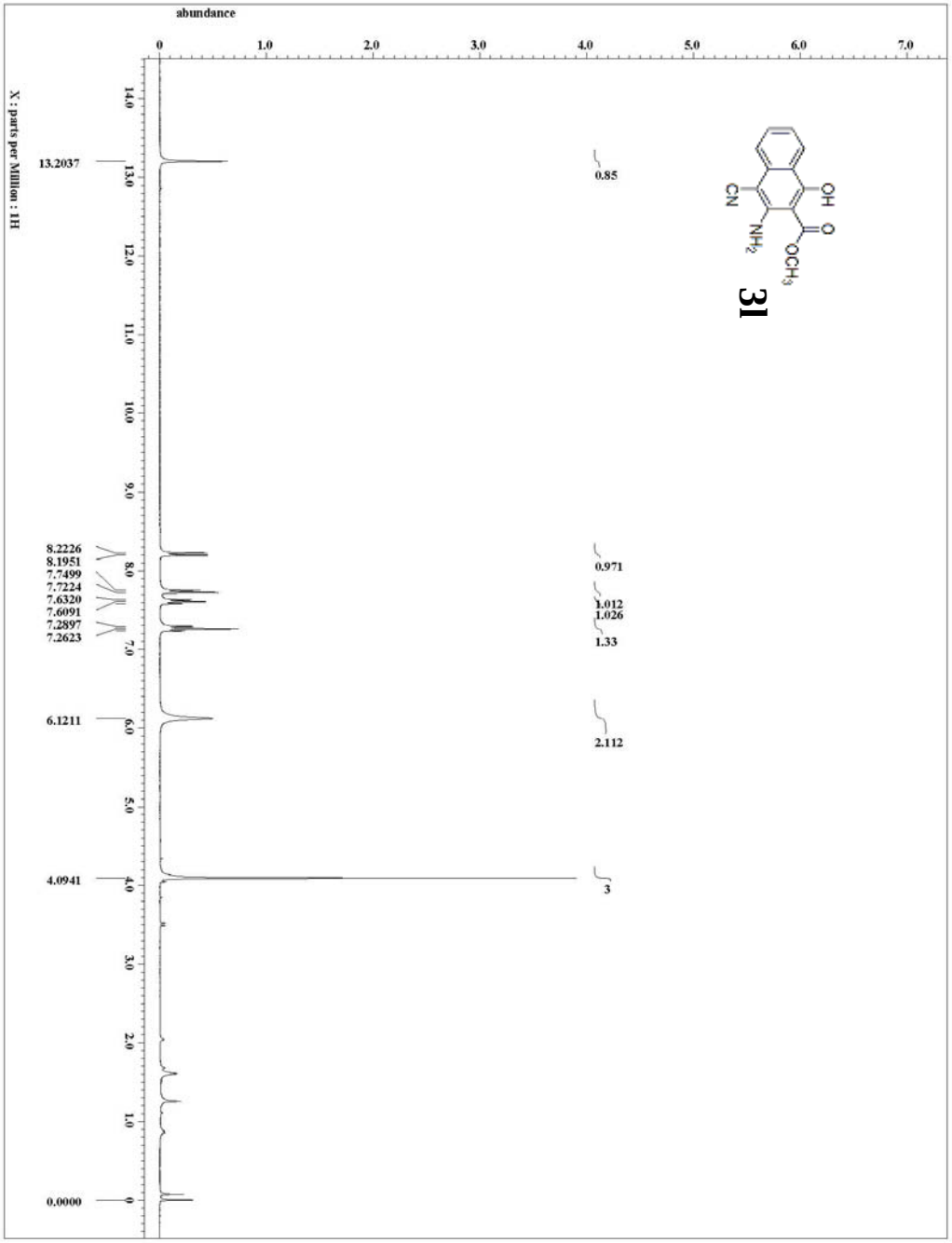
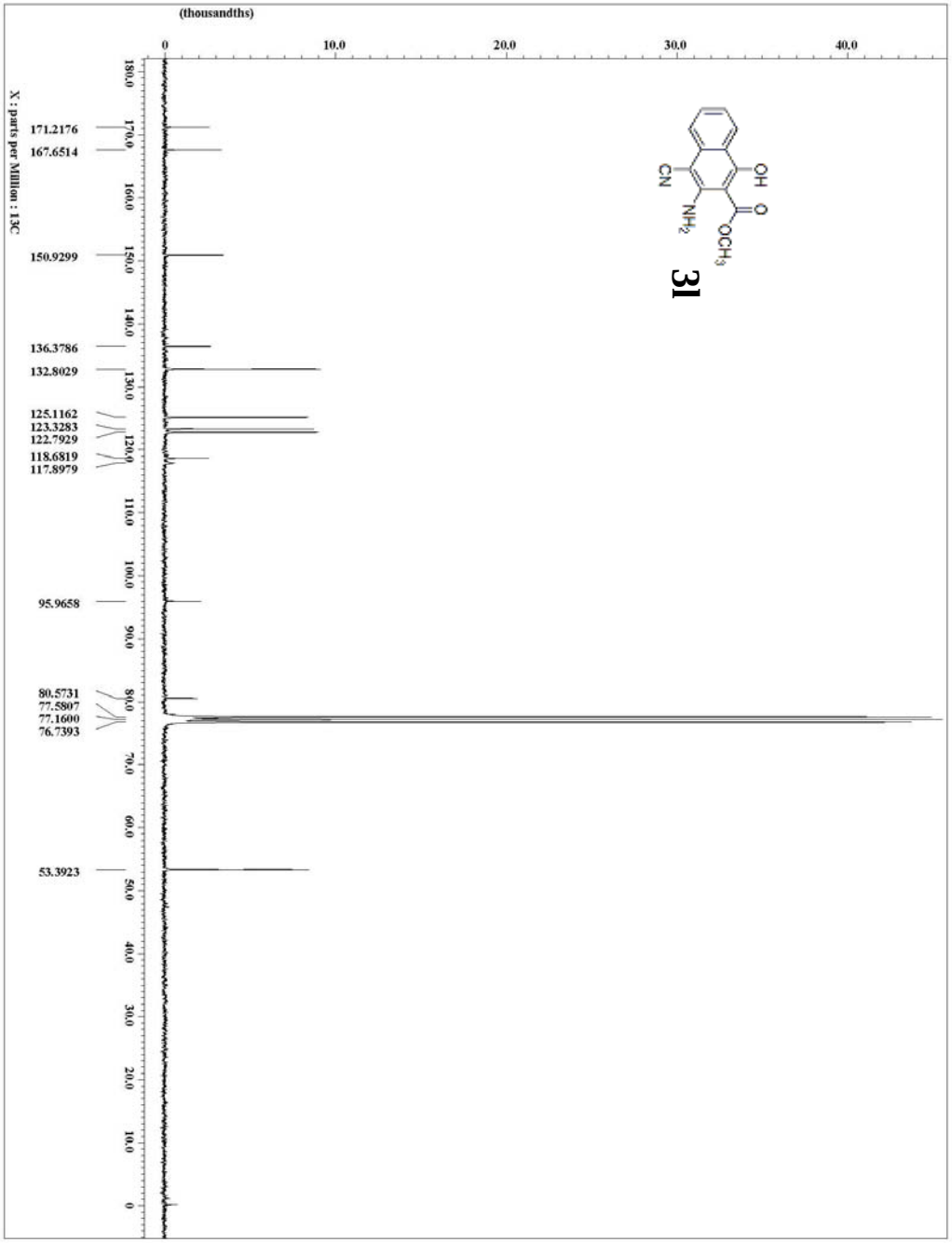
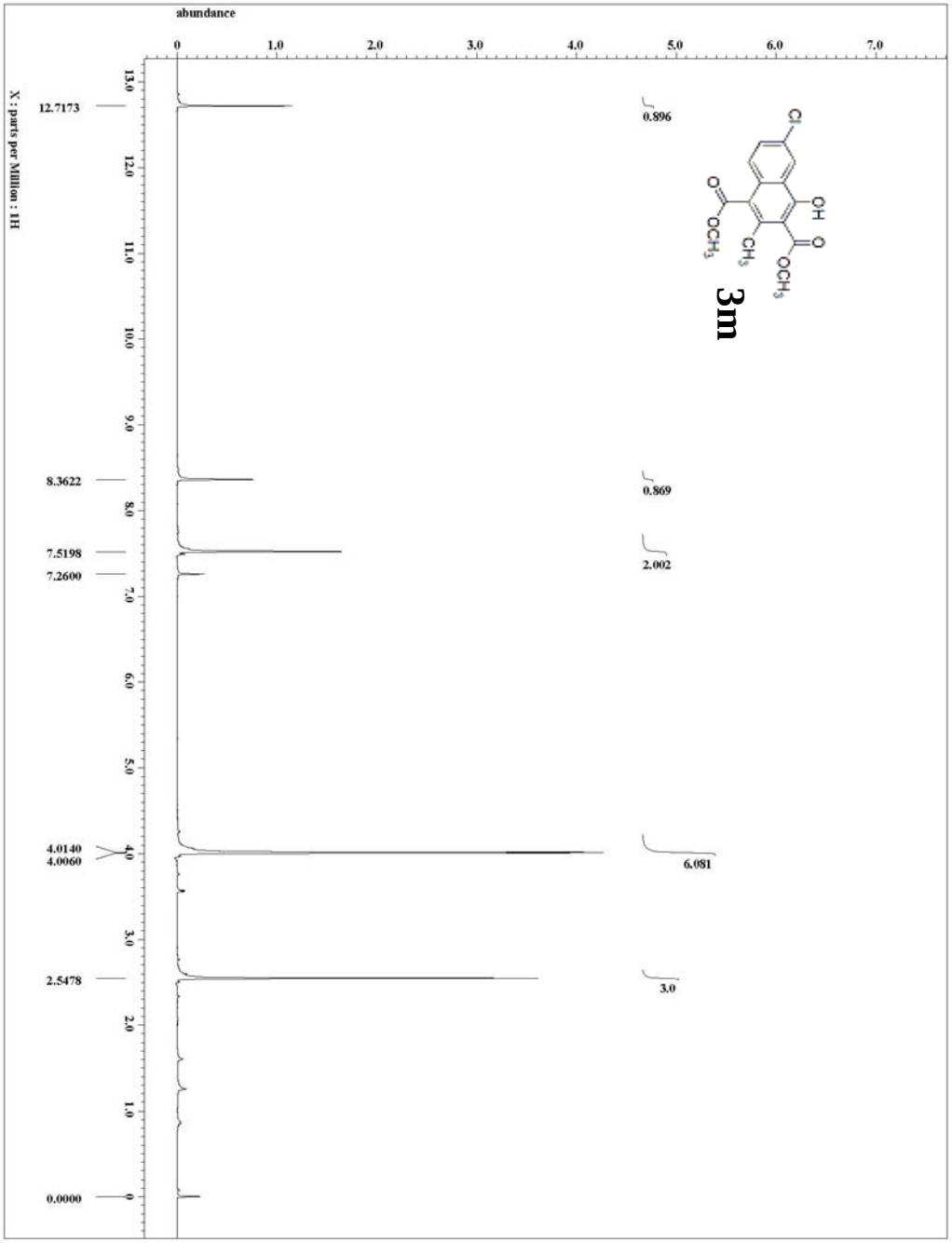
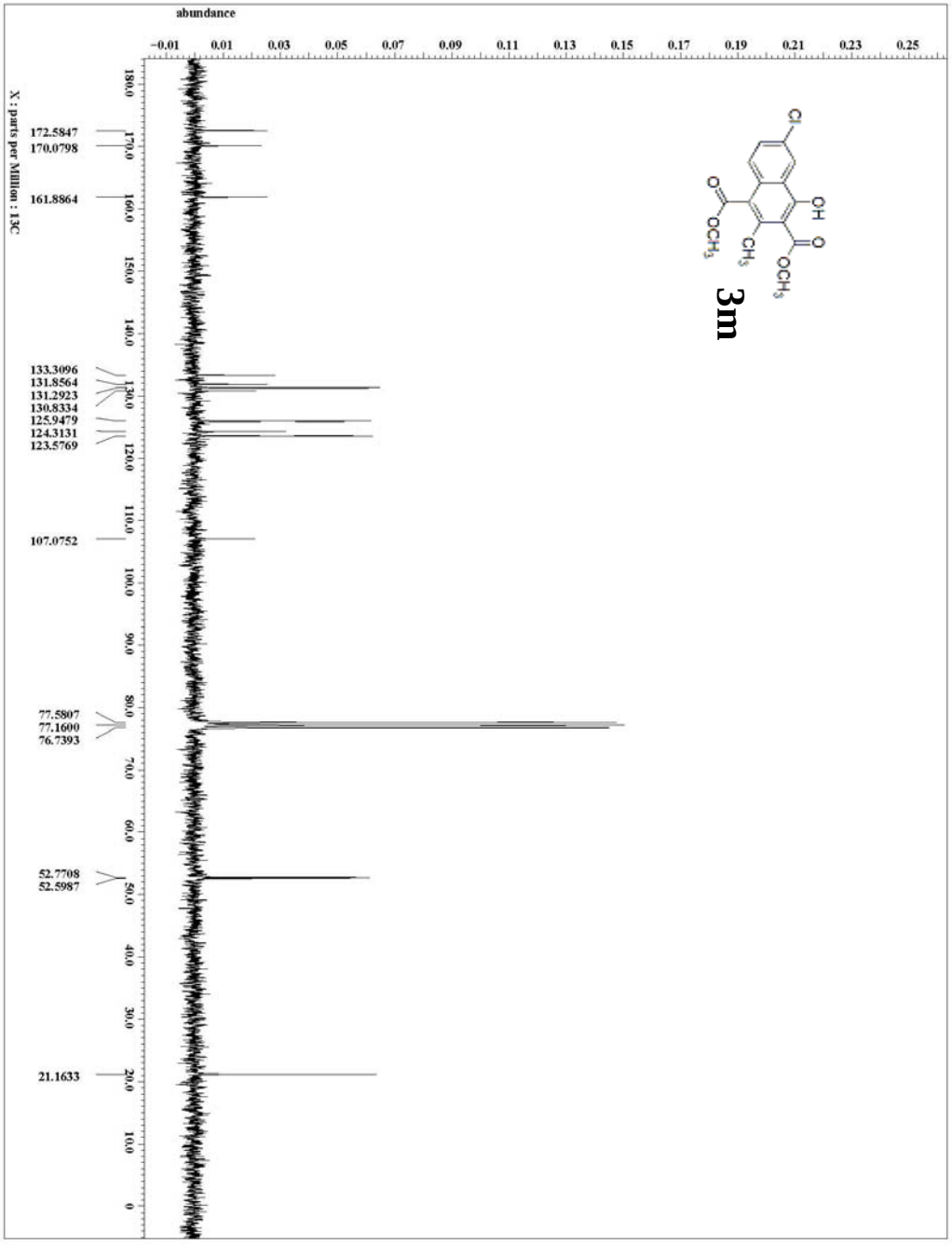
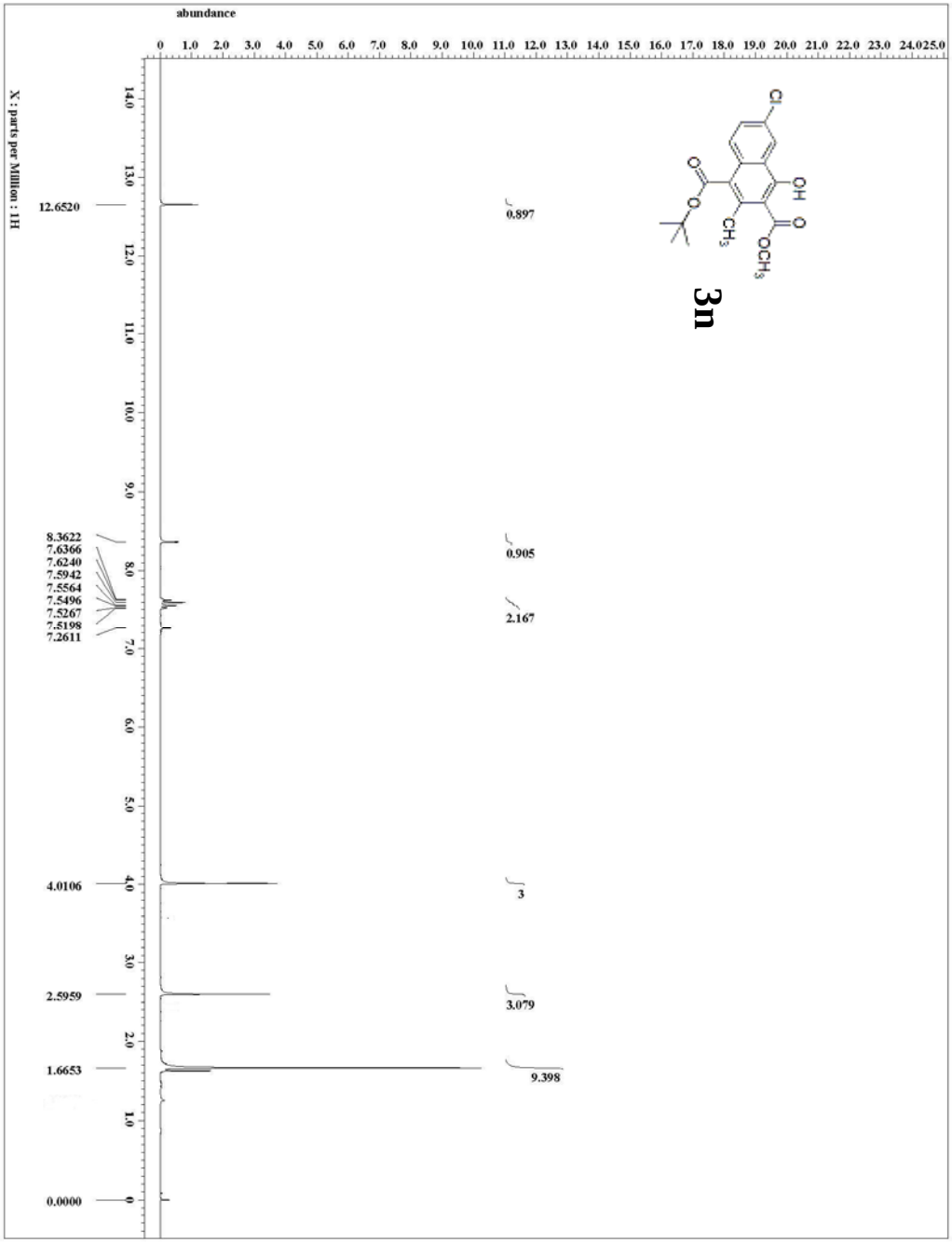
X_acq_time = 0.69206016[s]
X_angle = 30[deg]
X_atn = 7.46[dB]
X_pulse = 3.5[us]
Irr_atn = 16.79[dB]
Irr_atn_dec = 28.74704[dB]
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Relaxation_delay = 2[s]
Repetition_time = 2.69206016[s]
Solvent = CHLOROFORM-D
Spin_action = SPIN ON
Spin_state = SPIN ON
Spin_status = SPIN ON
Spin_gat = 1H [Hz]
Spin_gac_source = ATR
Sample_action = LOADED
Sample_state = LOAD
Sample_status = LOADED
Changer_sample = 0

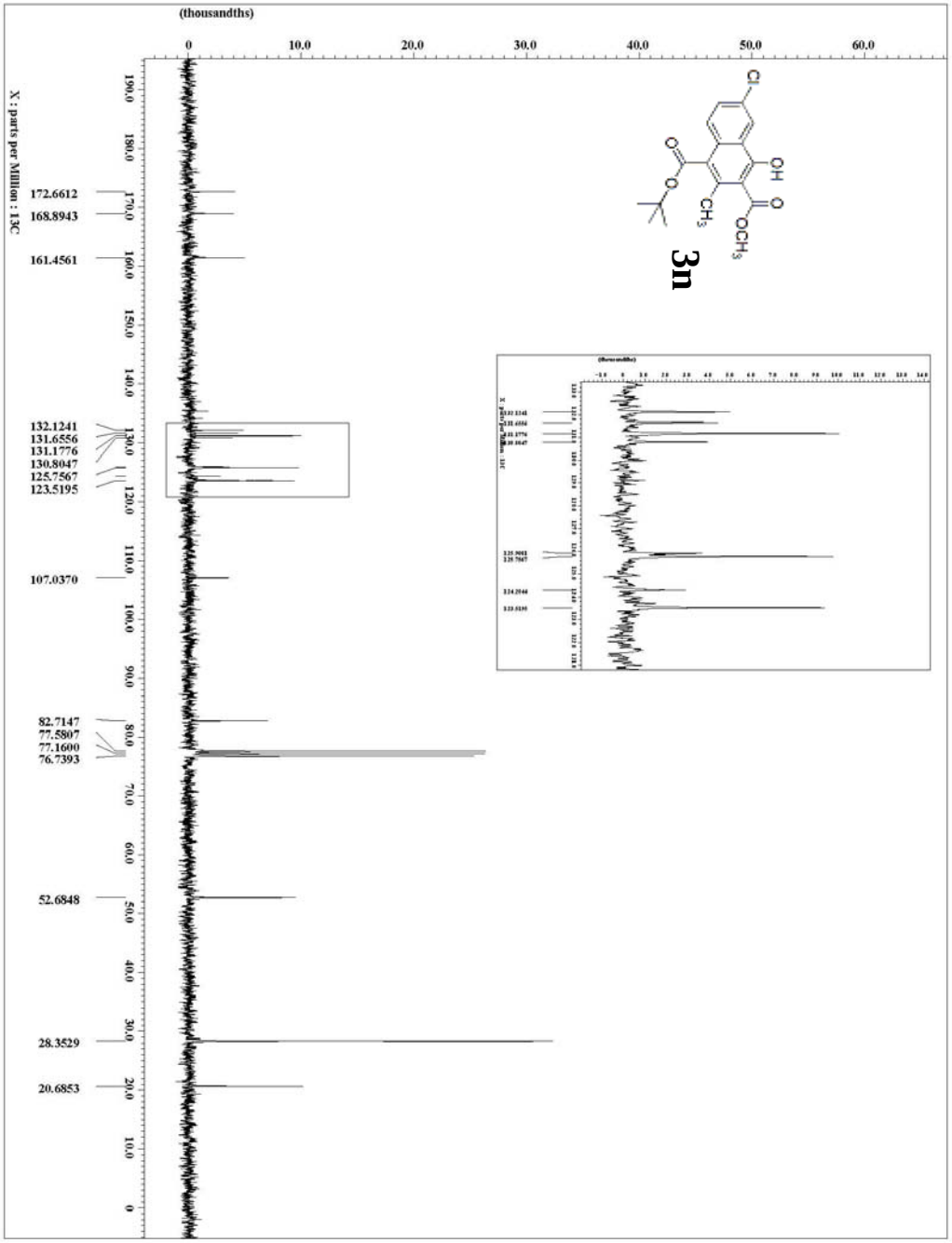

abundance
X : parts per Million : 1H
13.2037
8.2226
8.1951
7.7499
7.7224
7.6320
7.6091
7.2897
7.2623
6.1211
4.0941
0.0000
0.85
0.971
1.012
1.026
1.33
2.112
3
CN
OH
O
NH2
OCH3
31

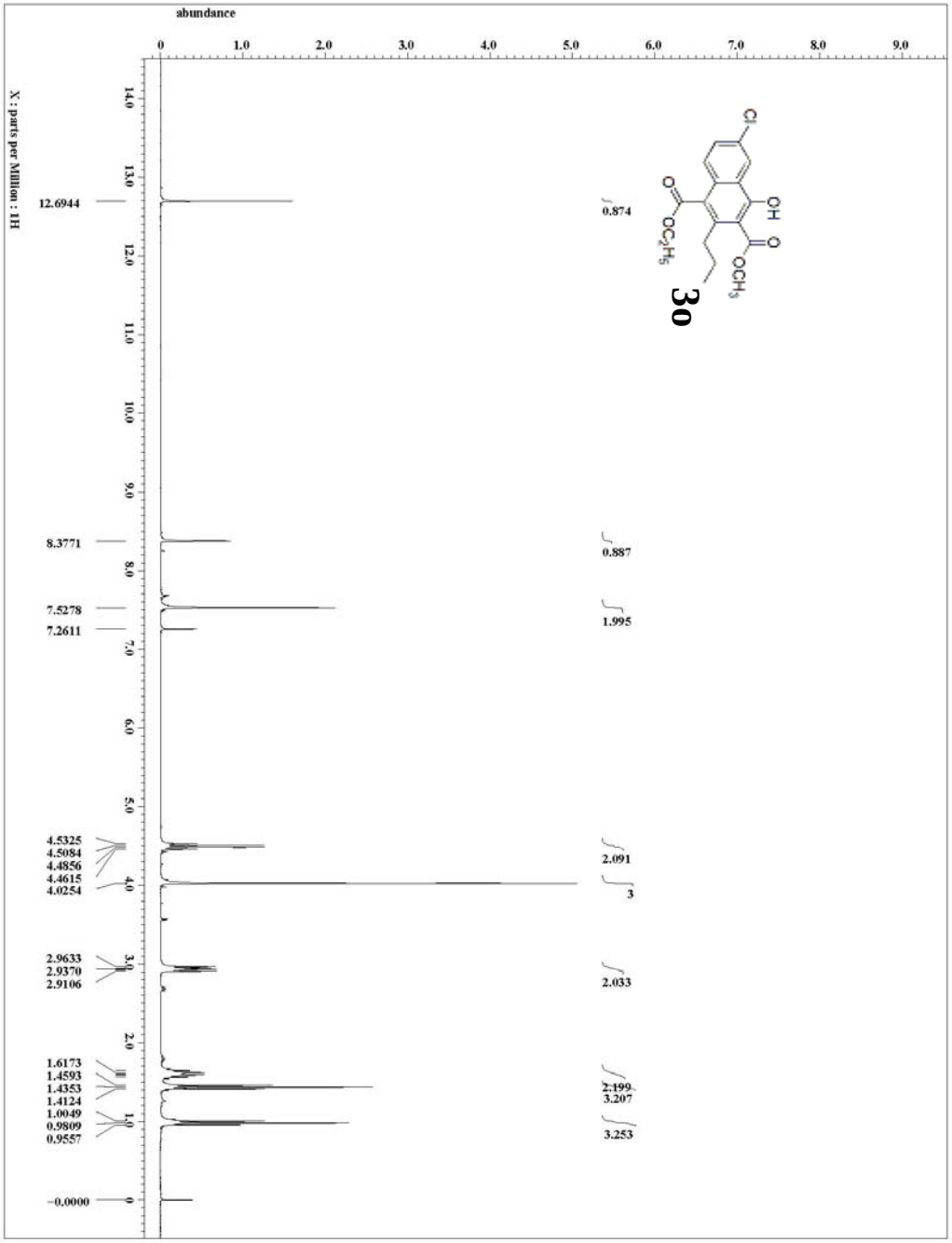

(thousandths)
0
10.0
20.0
30.0
40.0
X : parts per Million : 13C
171.2176
167.6514
150.9299
136.3786
132.8029
125.1162
123.3283
122.7929
118.6819
117.8979
95.9658
80.5731
77.5807
77.1600
76.7393
53.3923
CN
NH2
OH
O
OCH3
31

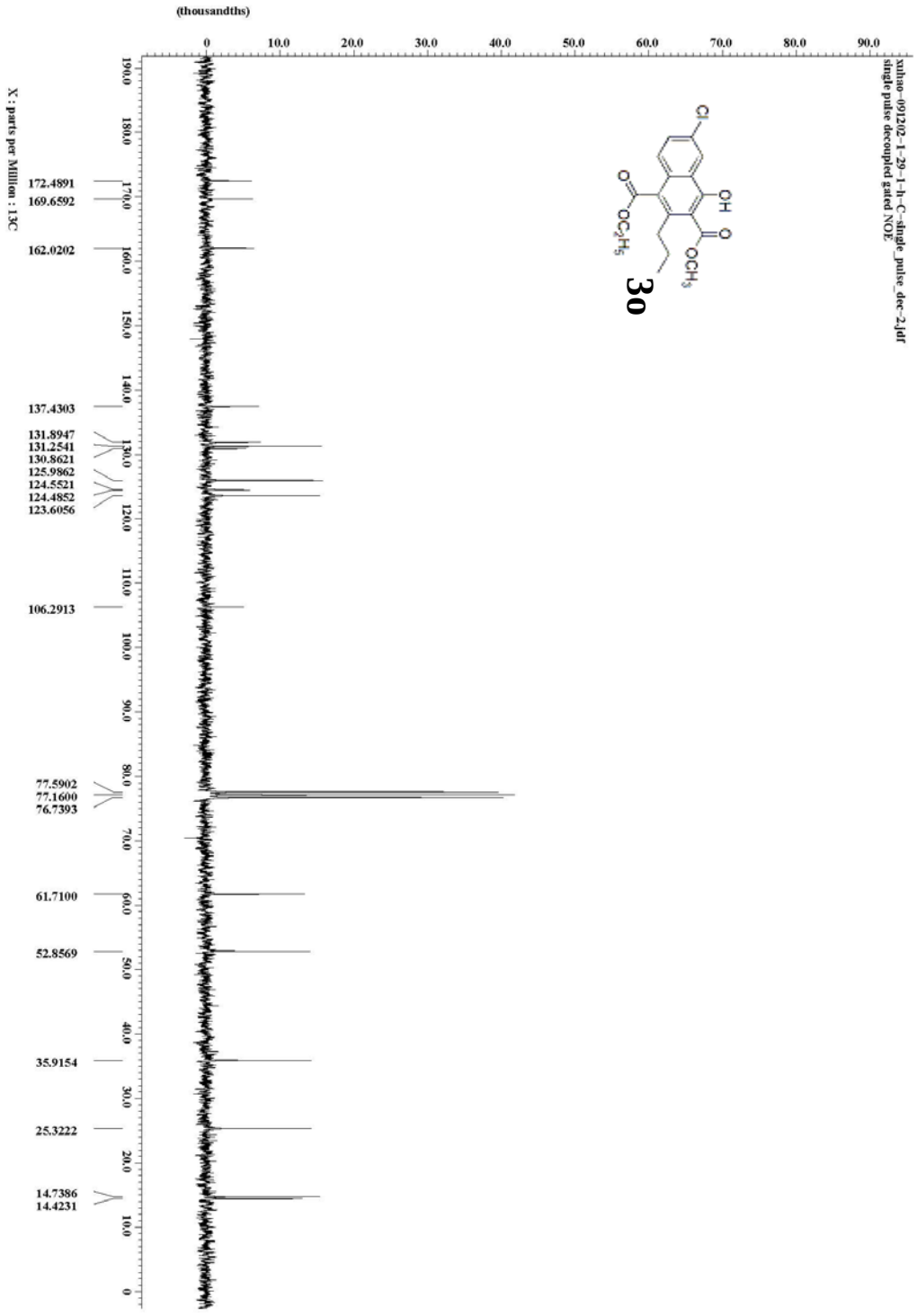

abundance
X : parts per Million : 1H
12.7173
8.3622
7.5198
7.2600
4.0140
4.0060
2.5478
0.0000
0.896
0.869
2.002
6.081
3.0
Cl
OH
O
OCH3
CH3
OCH3
3m

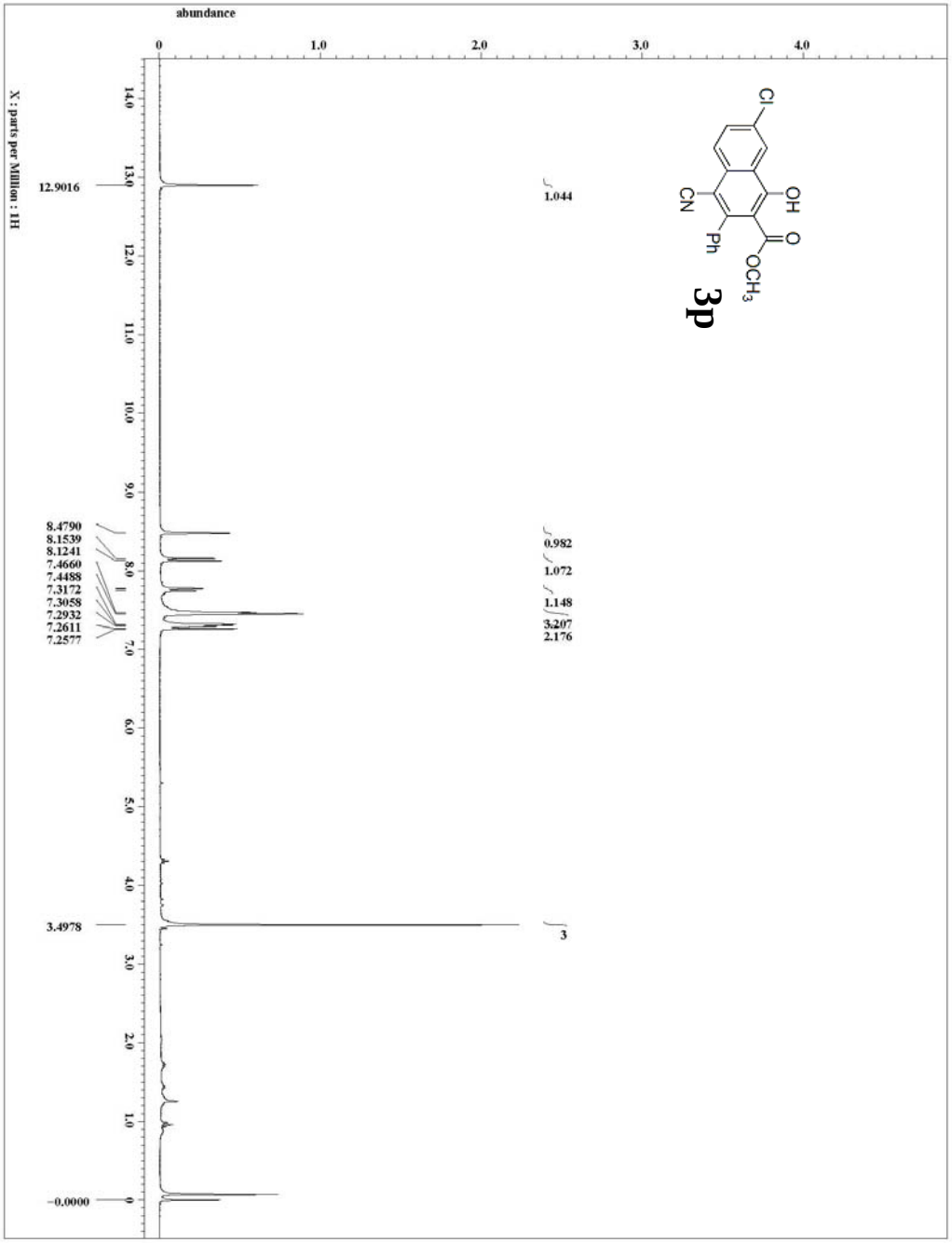

abundance
X : parts per Million : 13C
172.5847
170.0798
161.8864
133.3096
131.8564
131.2923
130.8334
125.9479
124.3131
123.5769
107.0752
77.5807
77.1600
76.7393
52.7708
52.5987
21.1633
3m

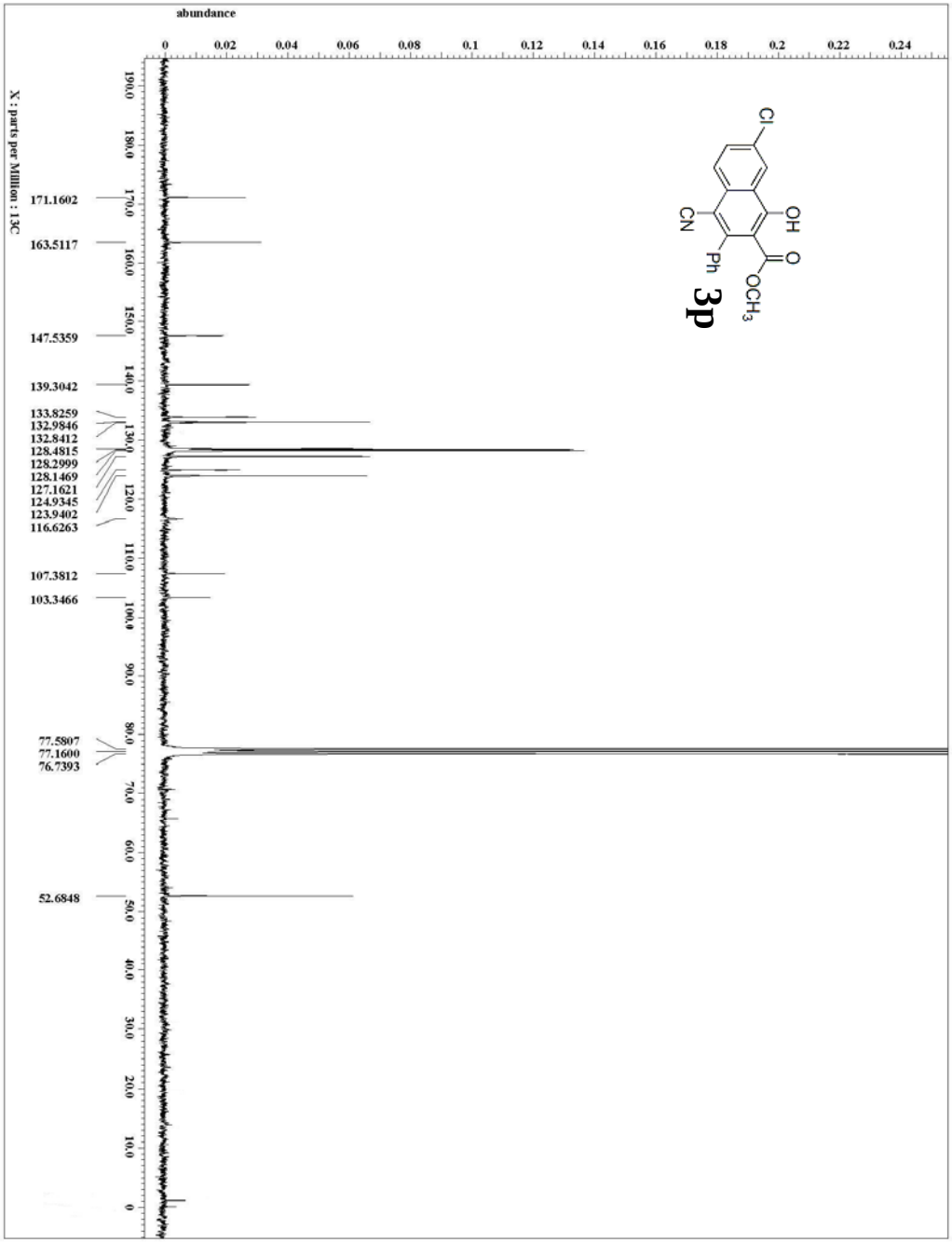

abundance
X : parts per Million : 1H
12.6520
8.3622
7.6366
7.6240
7.5942
7.5564
7.5496
7.5267
7.5198
7.2611
4.0106
2.5959
1.6653
0.0000
0.897
0.905
2.167
3
3.079
9.398
Cl
OH
O
CH3
OCH3
3n

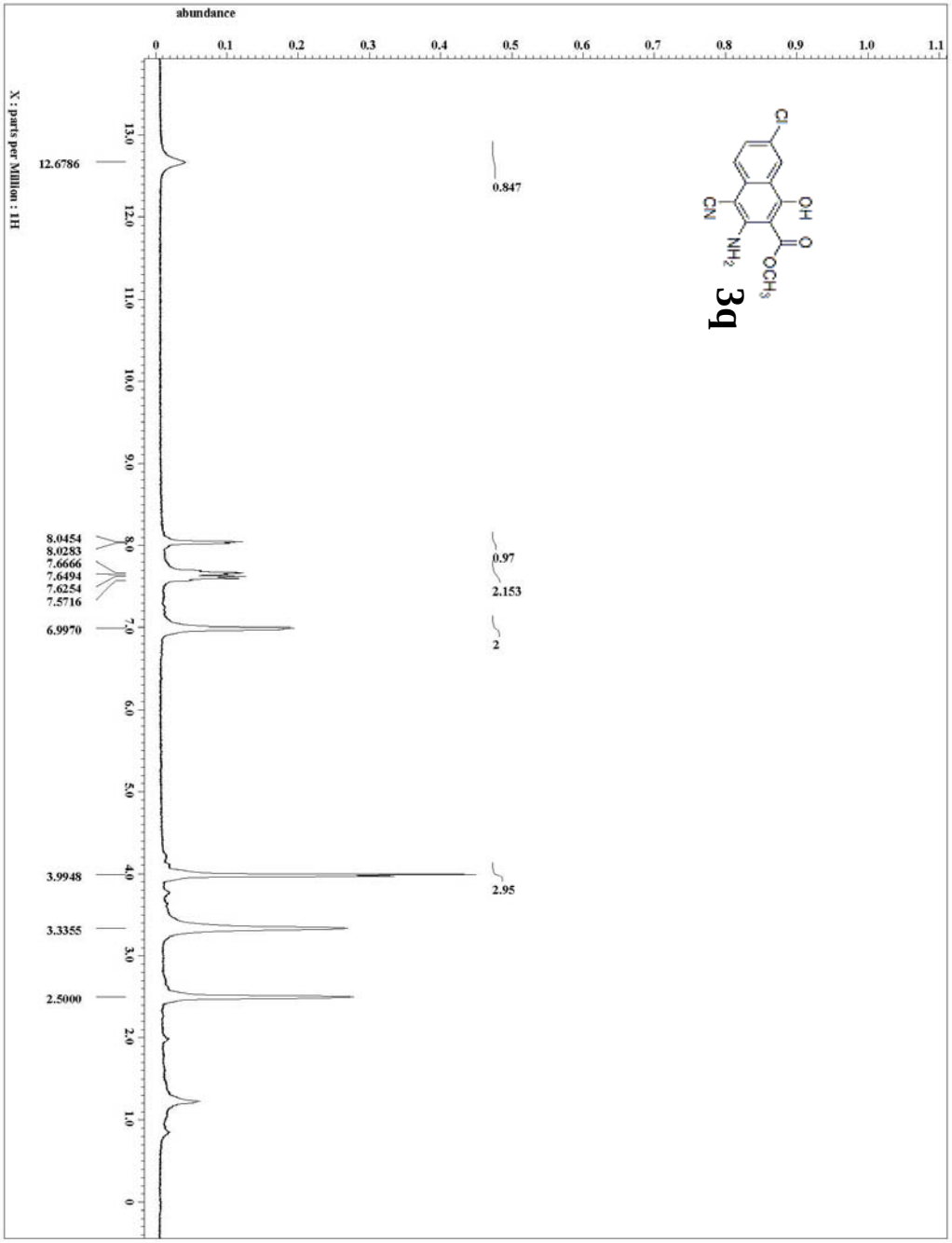

(thousandths)
X : parts per Million : 13C
172.6612
168.8943
161.4561
132.1241
131.6556
131.1776
130.8047
125.7567
123.5195
107.0370
82.7147
77.5807
77.1600
76.7393
52.6848
28.3529
20.6853
3n

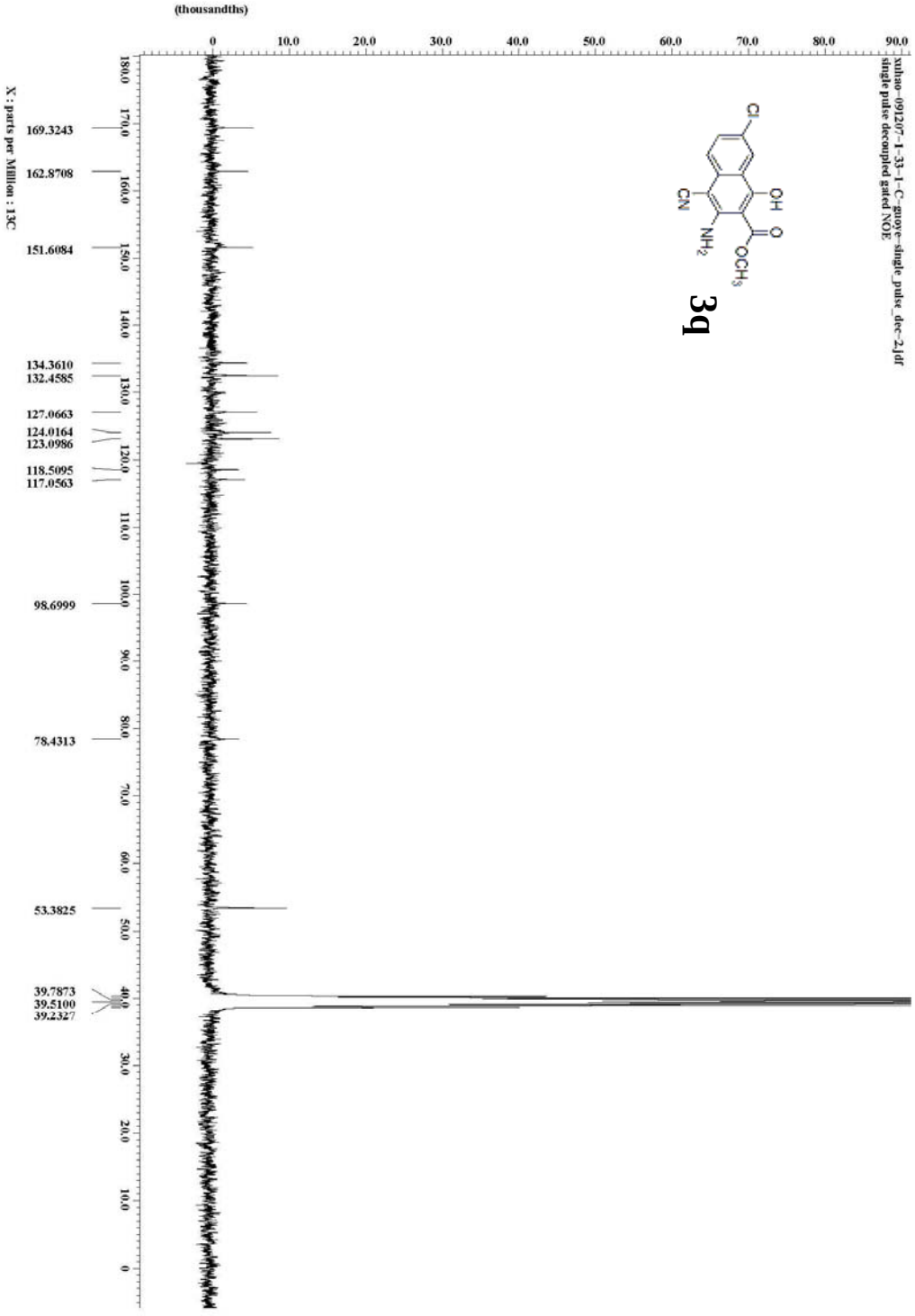

abundance
X : parts per Million : 1H
12.6944
8.3771
7.5278
7.2611
4.5325
4.5084
4.4856
4.4615
4.0254
2.9633
2.9370
2.9106
1.6173
1.4593
1.4353
1.4124
1.0049
0.9809
0.9557
-0.0000
0.874
0.887
1.995
2.091
3
2.033
2.199
3.207
3.253
Cl
OH
O
OC2H5
OCH3
30

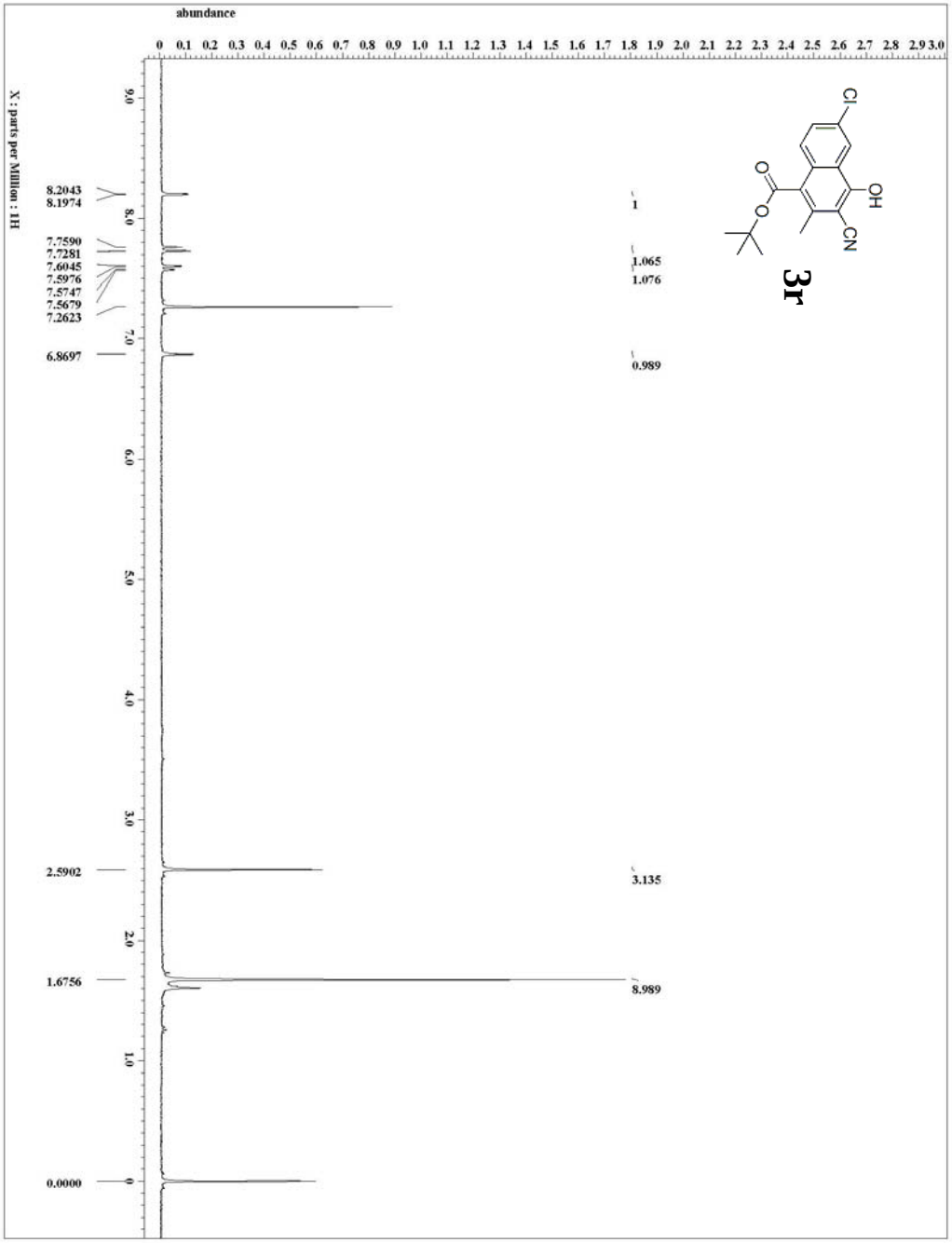

(thousandths)
0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
80.0
90.0
xuhao-091202-1-29-1-h-C-single_pulse_dec-2.jdf
single pulse decoupled gated NOE
X : parts per Million : 13C
172.4891
169.6592
162.0202
137.4303
131.8947
131.2541
130.8621
125.9862
124.5521
124.4852
123.6056
106.2913
77.5902
77.1600
76.7393
61.7100
52.8569
35.9154
25.3222
14.7386
14.4231
Cl
OH
O
OC2H5
OCH3
30

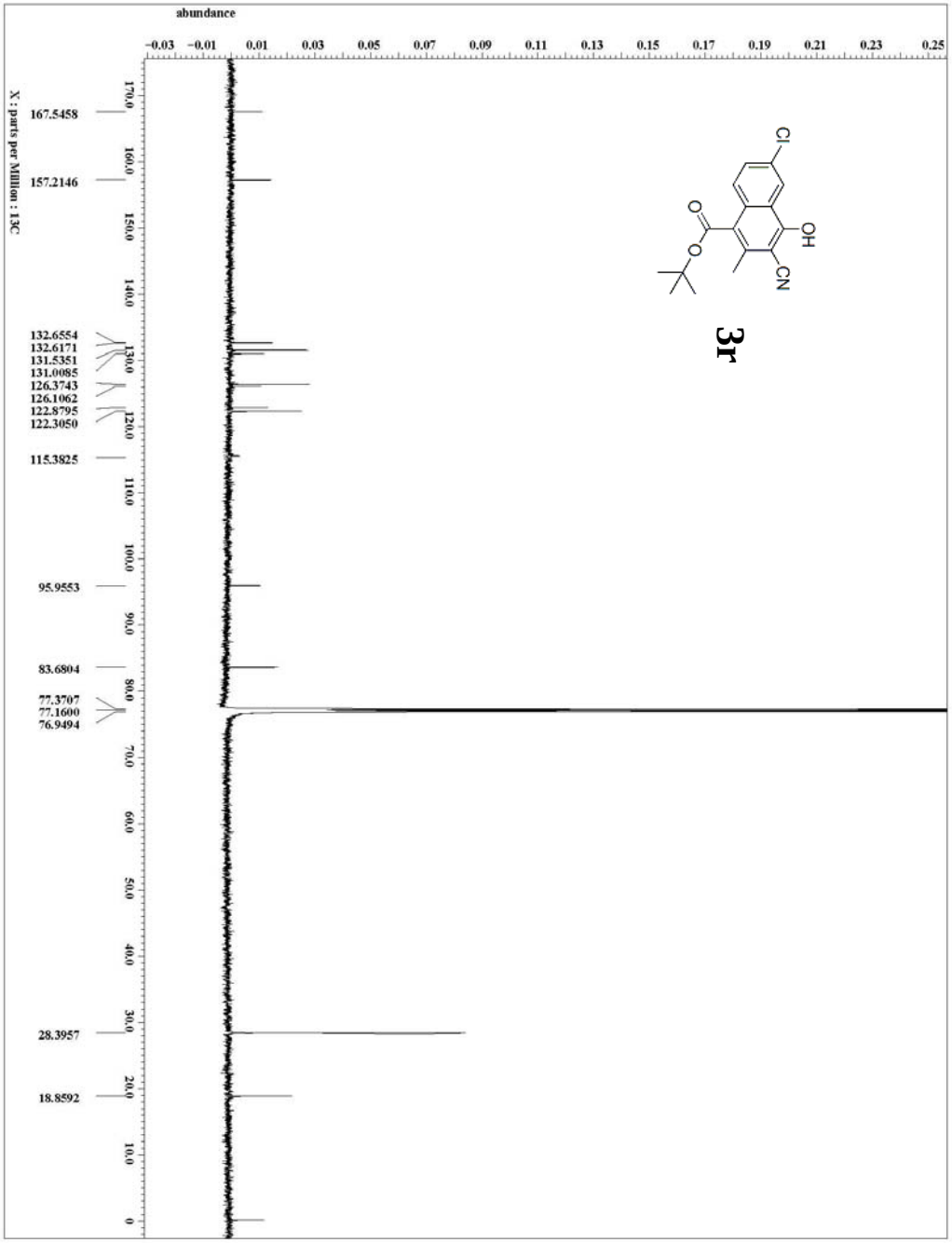

abundance
X : parts per Million : 1H
12.9016
8.4790
8.1539
8.1241
7.4660
7.4488
7.3172
7.3058
7.2932
7.2611
7.2577
3.4978
-0.0000
1.044
0.982
1.072
1.148
3.207
2.176
3
Cl
OH
O
CN
Ph
OCH3
3p

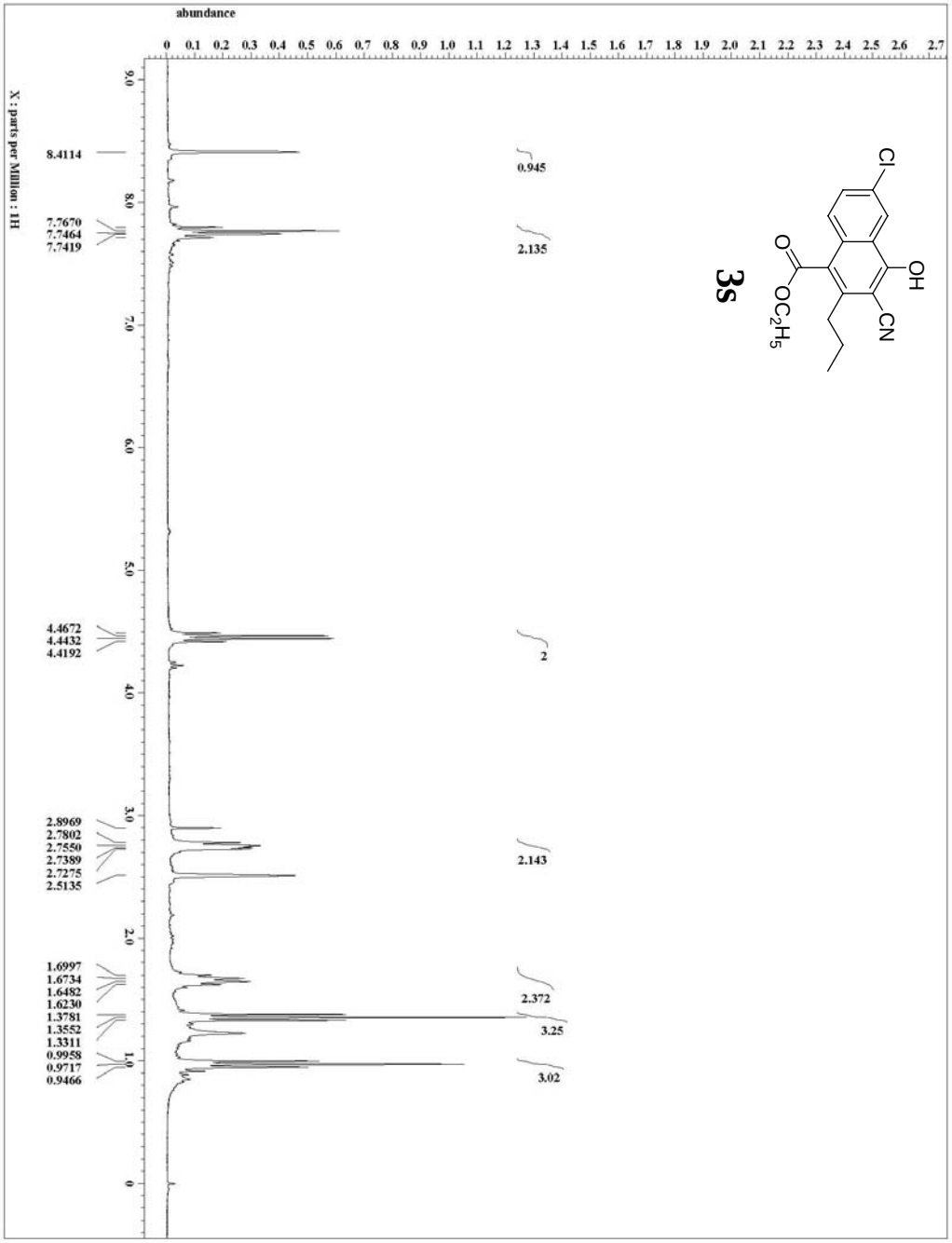

abundance
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.2
0.22
0.24
X : parts per Million : 13C
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
171.1602
163.5117
147.5359
139.3042
133.8259
132.9846
132.8412
128.4815
128.2999
128.1469
127.1621
124.9345
123.9402
116.6263
107.3812
103.3466
77.5807
77.1600
76.7393
52.6848
Cl
OH
O
CN
Ph
OCH3
3p

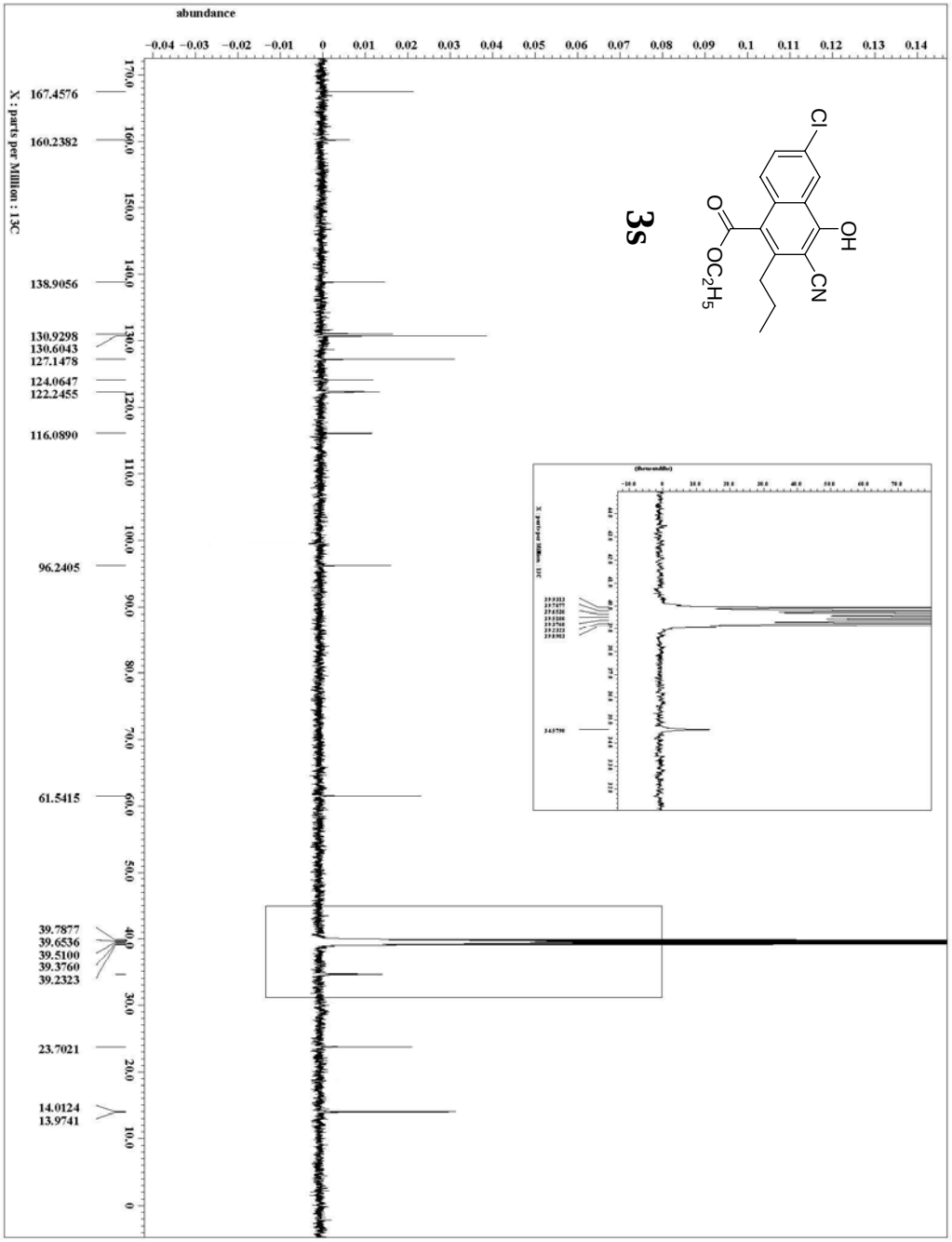

abundance
X : parts per Million : 1H
12.6786
8.0454
8.0283
7.6666
7.6494
7.6254
7.5716
6.9970
3.9948
3.3355
2.5000
0.847
0.97
2.153
2
2.95
Cl
OH
O
CN
NH2
OCH3
3g

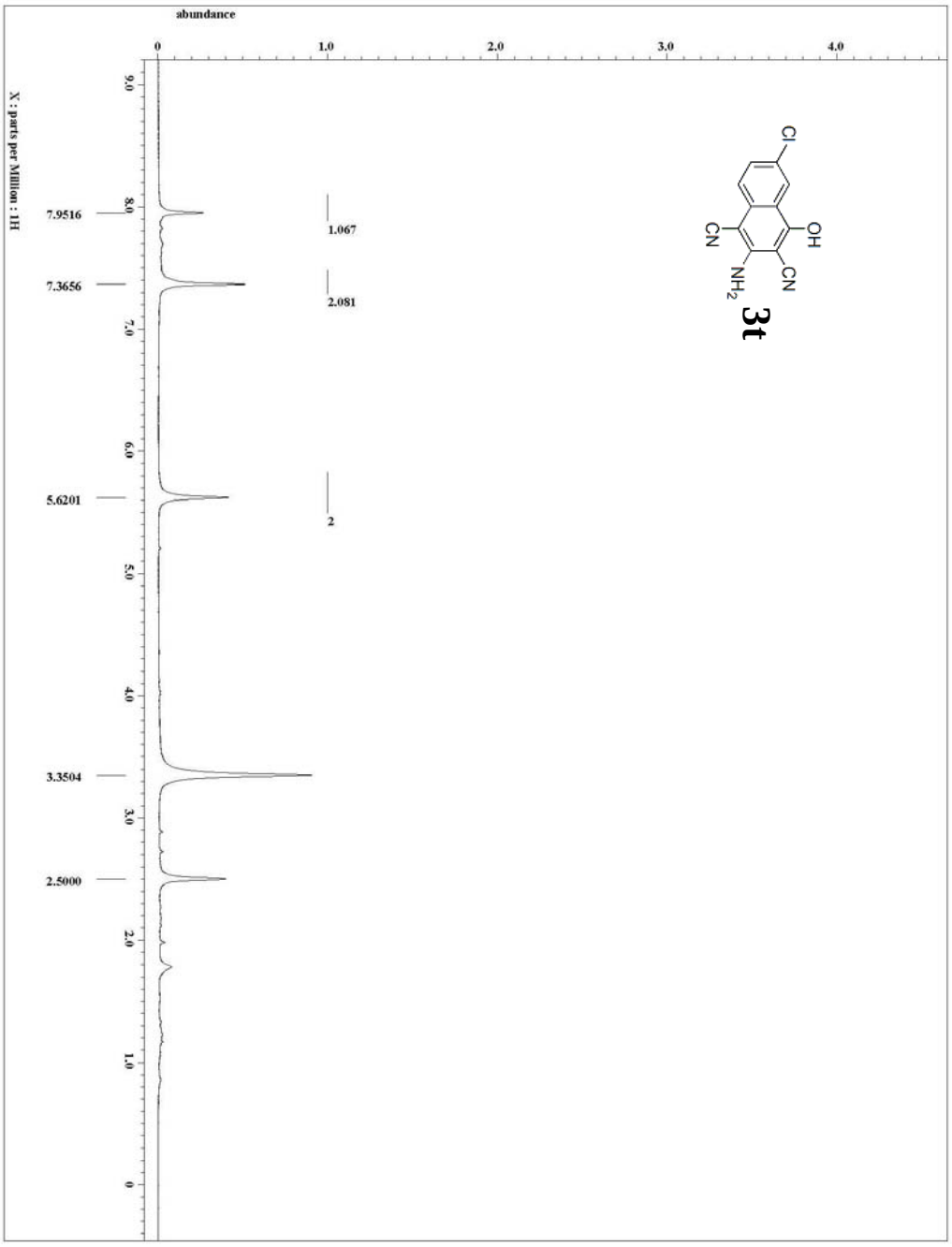

(thousandths)
0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
80.0
90.0
X : parts per Million : 13C
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
169.3243
162.8708
151.6084
134.3610
132.4585
127.0663
124.0164
123.0986
118.5095
117.0563
98.6999
78.4313
53.3825
39.7873
39.5100
39.2327
xuhao-091207-1-33-1-C-guoye-single_pulse_dec-2.jdf
single pulse decoupled gated NOE
Cl
OH
O
CN
NH2
OCH3
3g

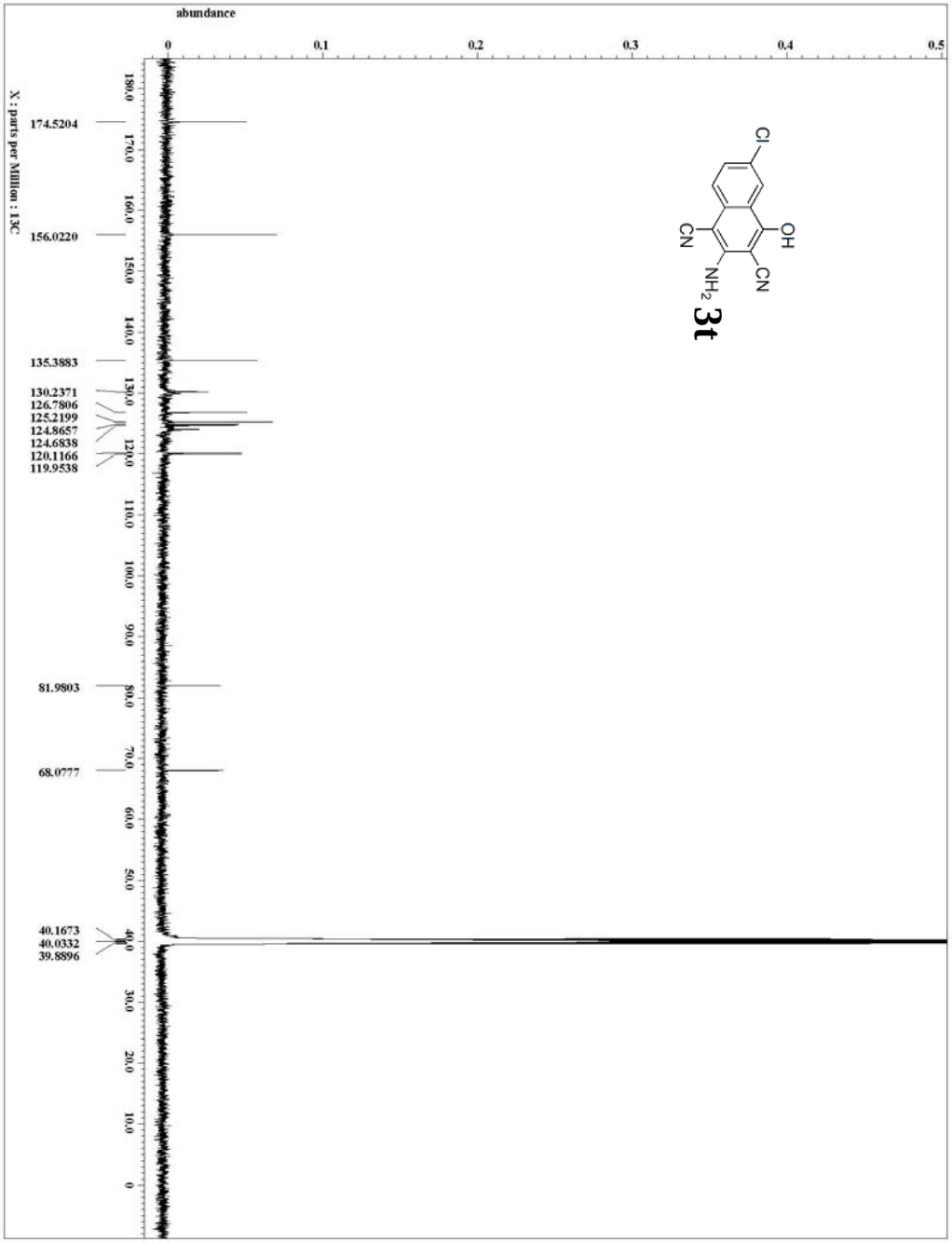

abundance
X : parts per Million : 1H
8.2043
8.1974
7.7590
7.7281
7.6045
7.5976
7.5747
7.5679
7.2623
6.8697
2.5902
1.6756
0.0000
1
1.065
1.076
0.989
3.135
8.989
Cl
OH
CN
O
O
3r


abundance
X : parts per Million : 13C
167.5458
157.2146
132.6554
132.6171
131.5351
131.0085
126.3743
126.1062
122.8795
122.3050
115.3825
95.9553
83.6804
77.3707
77.1600
76.9494
28.3957
18.8592
Cl
OH
CN
O
O
3r


abundance
X : parts per Million : 1H
8.4114
7.7670
7.7464
7.7419
4.4672
4.4432
4.4192
2.8969
2.7802
2.7550
2.7389
2.7275
2.5135
1.6997
1.6734
1.6482
1.6230
1.3781
1.3552
1.3311
0.9958
0.9717
0.9466
0.945
2.135
2
2.143
2.372
3.25
3.02
Cl
OH
CN
O
OC2H5
3s


abundance
X : parts per Million : 13C
167.4576
160.2382
138.9056
130.9298
130.6043
127.1478
124.0647
122.2455
116.0890
96.2405
61.5415
39.7877
39.6536
39.5100
39.3760
39.2323
23.7021
14.0124
13.9741
3s
Cl
OH
CN
O
OC2H5


abundance
0
1.0
2.0
3.0
4.0
X : parts per Million : 1H
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.9516
7.3656
5.6201
3.3504
2.5000
1.067
2.081
2
Cl
OH
CN
CN
NH2
3t


abundance
0
0.1
0.2
0.3
0.4
0.5
X : parts per Million : 13C
174.5204
156.0220
135.3883
130.2371
126.7806
125.2199
124.8657
124.6838
120.1166
119.9538
81.9803
68.0777
40.1673
40.0332
39.8596
Cl
OH
CN
CN
NH2
3t